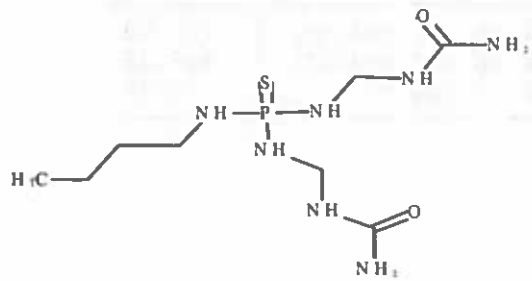


Experimental Database Structure Match: no data

SMILES : CCCCNP(=S)(NCNC(=O)N)NCNC(=O)N
CHEM :
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34

---------- SUMMARY MPBPWIN v1.43 ----------

Boiling Point: 480.00 deg C (Adapted Stein and Brown Method)

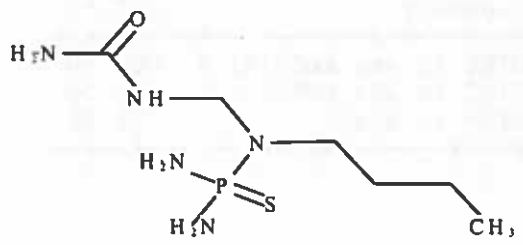
Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 166.61 deg C (Gold and Ogle Method)
Mean Melt Pt : 120.81 deg C (Joback; Gold,Ogle Methods)
Selected MP: 90.27 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 480.00 deg C (estimated))
(Using MP: 90.27 deg C (estimated))
VP: 5.99E-010 mm Hg (Antoine Method)
: 7.98E-008 Pa (Antoine Method)
VP: 2.06E-008 mm Hg (Modified Grain Method)
: 2.74E-006 Pa (Modified Grain Method)
VP: 4.2E-008 mm Hg (Mackay Method)
: 5.61E-006 Pa (Mackay Method)
Selected VP: 2.06E-008 mm Hg (Modified Grain Method)
: 2.74E-006 Pa (Modified Grain Method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-005 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	5	-CH2-	24.22	121.10
Group	3	>NH (nonring)	45.28	135.84
Group	2	-C(=O)NH2	230.39	460.78
Group	1	>P=S	100.00	100.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		1037.88
RESULT- corr		BOILING POINT in deg Kelvin		779.95
Special-Limit		BOILING POINT in deg Kelvin		753.16
		BOILING POINT in deg C		480.00

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	5	-CH2-	11.27	56.35
Group	3	>NH (nonring)	52.66	157.98
Group	2	-C(=O)NH2	230.00	460.00
Group	1	>P=S	-70.00	-70.00

*		Equation Constant	122.50
RESULT		MELTING POINT in deg Kelvin	721.73
Special-limit		MELTING POINT in deg Kelvin	348.16
		MELTING POINT in deg C	75.00



Experimental Database Structure Match: no data

SMILES : NC(=O)NCN(CCCC)P(=S)(N)N
CHEM :
MOL FOR: C6 H18 N5 O1 P1 S1
MOL WT : 239.28

---------- SUMMARY MPBPWIN v1.43 ----------

Boiling Point: 391.46 deg C (Adapted Stein and Brown Method)

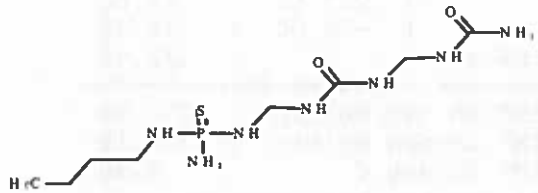
Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 114.91 deg C (Gold and Ogle Method)
Mean Melt Pt : 94.96 deg C (Joback; Gold,Ogle Methods)
Selected MP: 84.98 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 391.46 deg C (estimated))
(Using MP: 84.98 deg C (estimated))
VP: 8.85E-007 mm Hg (Antoine Method)
: 0.000118 Pa (Antoine Method)
VP: 3.57E-006 mm Hg (Modified Grain Method)
: 0.000475 Pa (Modified Grain Method)
VP: 6.98E-006 mm Hg (Mackay Method)
: 0.000931 Pa (Mackay Method)
Selected VP: 3.57E-006 mm Hg (Modified Grain Method)
: 0.000475 Pa (Modified Grain Method)
Subcooled liquid VP: 1.34E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.00179 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	4	-CH2-	24.22	96.88
Group	2	-NH2	61.98	123.96
Group	1	>N-	25.78	25.78
Group	1	-C(=O)NH2	230.39	230.39
Group	1	>P=S	100.00	100.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		797.17
RESULT- corr		BOILING POINT in deg Kelvin		664.62
		BOILING POINT in deg C		391.46

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	4	-CH2-	11.27	45.08
Group	2	-NH2	66.89	133.78
Group	1	>N-	48.84	48.84
Group	1	-C(=O)NH2	230.00	230.00

Group *	1	>P=S Equation Constant	-70.00	-70.00 122.50
RESULT		MELTING POINT in deg Kelvin		505.10
Special-limit		MELTING POINT in deg Kelvin		348.16
		MELTING POINT in deg C		75.00



Experimental Database Structure Match: no data

SMILES : CCCCNP(=S)(N)NCNC(=O)NCNC(=O)N
CHEM :
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34

---------- SUMMARY MPBPWIN v1.43 ----------

Boiling Point: 480.00 deg C (Adapted Stein and Brown Method)

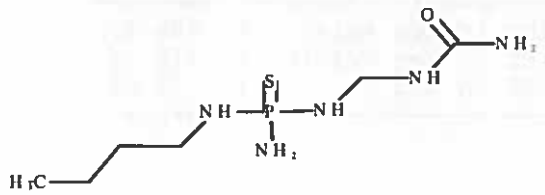
Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 166.61 deg C (Gold and Ogle Method)
Mean Melt Pt : 120.81 deg C (Joback; Gold,Ogle Methods)
Selected MP: 90.27 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 480.00 deg C (estimated))
(Using MP: 90.27 deg C (estimated))
VP: 5.99E-010 mm Hg (Antoine Method)
: 7.98E-008 Pa (Antoine Method)
VP: 2.06E-008 mm Hg (Modified Grain Method)
: 2.74E-006 Pa (Modified Grain Method)
VP: 4.2E-008 mm Hg (Mackay Method)
: 5.61E-006 Pa (Mackay Method)
Selected VP: 2.06E-008 mm Hg (Modified Grain Method)
: 2.74E-006 Pa (Modified Grain Method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-005 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	5	-CH2-	24.22	121.10
Group	1	-NH2	61.98	61.98
Group	2	>NH (nonring)	45.28	90.56
Group	1	-C(=O)NH2	230.39	230.39
Group	1	-C(=O)NH-	225.09	225.09
Group	1	>P=S	100.00	100.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		1049.28
RESULT- corr		BOILING POINT in deg Kelvin		785.41
Special-Limit		BOILING POINT in deg Kelvin		753.16
		BOILING POINT in deg C		480.00

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	5	-CH2-	11.27	56.35
Group	1	-NH2	66.89	66.89

Group	2	>NH (nonring)	52.66	105.32
Group	1	-C(=O)NH2	230.00	230.00
Group	1	-C(=O)NH-	225.00	225.00
Group	1	>P=S	-70.00	-70.00
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		730.96
Special-limit		MELTING POINT in deg Kelvin		348.16
		MELTING POINT in deg C		75.00



Experimental Database Structure Match: no data

SMILES : CCCCNP(=S)(N)NCNC(=O)N
CHEM :
MOL FOR: C6 H18 N5 O1 P1 S1
MOL WT : 239.28

---------- SUMMARY MPBPWIN v1.43 ----------

Boiling Point: 392.81 deg C (Adapted Stein and Brown Method)

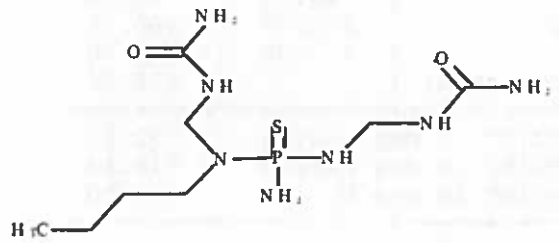
Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 115.70 deg C (Gold and Ogle Method)
Mean Melt Pt : 95.35 deg C (Joback; Gold,Ogle Methods)
Selected MP: 85.17 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 392.81 deg C (estimated))
(Using MP: 85.17 deg C (estimated))
VP: 7.98E-007 mm Hg (Antoine Method)
: 0.000106 Pa (Antoine Method)
VP: 3.29E-006 mm Hg (Modified Grain Method)
: 0.000439 Pa (Modified Grain Method)
VP: 6.46E-006 mm Hg (Mackay Method)
: 0.000861 Pa (Mackay Method)
Selected VP: 3.29E-006 mm Hg (Modified Grain Method)
: 0.000439 Pa (Modified Grain Method)
Subcooled liquid VP: 1.24E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.00166 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	4	-CH2-	24.22	96.88
Group	1	-NH2	61.98	61.98
Group	2	>NH (nonring)	45.28	90.56
Group	1	-C(=O)NH2	230.39	230.39
Group	1	>P=S	100.00	100.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		799.97
RESULT- corr		BOILING POINT in deg Kelvin		665.97
		BOILING POINT in deg C		392.81

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	4	-CH2-	11.27	45.08
Group	1	-NH2	66.89	66.89
Group	2	>NH (nonring)	52.66	105.32
Group	1	-C(=O)NH2	230.00	230.00

Group *	1	>P=S	-70.00	-70.00
		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		494.69
Special-limit		MELTING POINT in deg Kelvin		348.16
		MELTING POINT in deg C		75.00



Experimental Database Structure Match: no data

SMILES : CCCCN(CNC(=O)N)P(=S)(N)NCNC(=O)N
CHEM :
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34
---------- SUMMARY MPBPWIN v1.43 ----------

Boiling Point: 480.00 deg C (Adapted Stein and Brown Method)

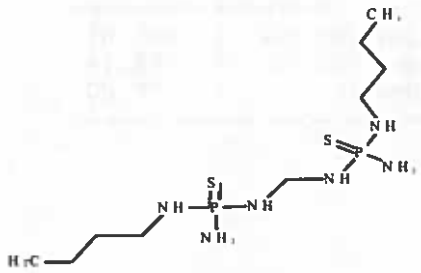
Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 166.61 deg C (Gold and Ogle Method)
Mean Melt Pt : 120.81 deg C (Joback; Gold,Ogle Methods)
Selected MP: 90.27 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 480.00 deg C (estimated))
(Using MP: 90.27 deg C (estimated))
VP: 5.99E-010 mm Hg (Antoine Method)
: 7.98E-008 Pa (Antoine Method)
VP: 2.06E-008 mm Hg (Modified Grain Method)
: 2.74E-006 Pa (Modified Grain Method)
VP: 4.2E-008 mm Hg (Mackay Method)
: 5.61E-006 Pa (Mackay Method)
Selected VP: 2.06E-008 mm Hg (Modified Grain Method)
: 2.74E-006 Pa (Modified Grain Method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-005 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	5	-CH2-	24.22	121.10
Group	1	-NH2	61.98	61.98
Group	1	>NH (nonring)	45.28	45.28
Group	1	>N-	25.78	25.78
Group	2	-C(=O)NH2	230.39	460.78
Group	1	>P=S	100.00	100.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		1035.08
RESULT- corr		BOILING POINT in deg Kelvin		778.61
Special-Limit		BOILING POINT in deg Kelvin		753.16
		BOILING POINT in deg C		480.00

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	5	-CH2-	11.27	56.35
Group	1	-NH2	66.89	66.89

Group	1	>NH (nonring)	52.66	52.66
Group	1	>N-	48.84	48.84
Group	2	-C(=O)NH2	230.00	460.00
Group	1	>P=S	-70.00	-70.00
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		732.14
Special-limit		MELTING POINT in deg Kelvin		348.16
		MELTING POINT in deg C		75.00



Experimental Database Structure Match: no data

SMILES : CCCCNP(=S)(N)NCNP(=S)(N)NCCCC
CHEM :
MOL FOR: C9 H28 N6 P2 S2
MOL WT : 346.43

---------- SUMMARY MPBPWIN v1.43 ----------

Boiling Point: 448.76 deg C (Adapted Stein and Brown Method)

Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 148.37 deg C (Gold and Ogle Method)
Mean Melt Pt : 111.68 deg C (Joback; Gold,Ogle Methods)
Selected MP: 87.23 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 448.76 deg C (estimated))
(Using MP: 87.23 deg C (estimated))
VP: 9.5E-009 mm Hg (Antoine Method)
: 1.27E-006 Pa (Antoine Method)
VP: 1.33E-007 mm Hg (Modified Grain Method)
: 1.78E-005 Pa (Modified Grain Method)
VP: 2.69E-007 mm Hg (Mackay Method)
: 3.58E-005 Pa (Mackay Method)
Selected VP: 1.33E-007 mm Hg (Modified Grain Method)
: 1.78E-005 Pa (Modified Grain Method)
Subcooled liquid VP: 5.28E-007 mm Hg (25 deg C, Mod-Grain method)
: 7.03E-005 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	7	-CH2-	24.22	169.54
Group	2	-NH2	61.98	123.96
Group	4	>NH (nonring)	45.28	181.12
Group	2	>P=S	100.00	200.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		916.76
RESULT- corr		BOILING POINT in deg Kelvin		721.92
		BOILING POINT in deg C		448.76

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH3	-5.10	-10.20
Group	7	-CH2-	11.27	78.89
Group	2	-NH2	66.89	133.78
Group	4	>NH (nonring)	52.66	210.64
Group	2	>P=S	-70.00	-140.00
*		Equation Constant		122.50

RESULT	MELTING POINT in deg Kelvin	395.61
Special-limit	MELTING POINT in deg Kelvin	348.16
	MELTING POINT in deg C	75.00