Thiourea, N,N'-dibutyl-

Other names:	Urea, 1,3-dibutyl-2-thio-
	N,N'-Dibutylthiourea
	Pennzone B
	1,3-Dibutyl-2-thiourea
	1,3-Dibutylthiourea
	N,N'-di-Normal-butylthiourea
	N,N'-di-n-Butylthiourea
	1,3-di-n-Butylthiourea
	Urea, 1,3-di-N-butyl-2-thio-
	USAF EK-2138
	1,3-Di-N-butyl-2-thiourea
	Thiate U
	NSC 3735
	1,3-Butylthiourea
Inchi:	InChI=1S/C9H20N2S/c1-3-5-7-10-9(12)11-8-6-4-2/h3-8H2,1-2H3,(H2,10,11,12)
InchiKey:	KFFQABQEJATQAT-UHFFFAOYSA-N
Formula:	C9H20N2S
SMILES:	CCCCNC(=S)NCCCC
Mol. weight [g/mol]:	188.33
CAS:	109-46-6

Physical Properties

Property code	Value	Unit	Source
gf	320.74	kJ/mol	Joback Method
hf	24.35	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hsub	141.00 ± 2.00	kJ/mol	NIST Webbook
hsub	137.00 ± 3.00	kJ/mol	NIST Webbook
hvap	55.23	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.051		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	575.70	K	Joback Method
tc	767.51	K	Joback Method
tf	337.50 ± 0.10	K	NIST Webbook
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.66	J/mol×K	575.70	Joback Method
cpg	428.62	J/mol×K	607.67	Joback Method
cpg	441.84	J/mol×K	639.64	Joback Method
cpg	454.35	J/mol×K	671.61	Joback Method
cpg	466.20	J/mol×K	703.57	Joback Method
cpg	477.43	J/mol×K	735.54	Joback Method
cpg	488.08	J/mol×K	767.51	Joback Method
hfust	28.34	kJ/mol	338.00	NIST Webbook
hvapt	105.00 ± 2.00	kJ/mol	385.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109466&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume