Allylthiourea

Other names:	Thiourea, 2-propenyl-
	Urea, 1-allyl-2-thio-
	Allylthiocarbamide
	Aminosin
	N-Allylthiourea
	Rhodallin
	Rhodalline
	Thiosinamin
	Thiosinamine
	U 19571
	1-Allyl-2-thiourea
	1-Allylthiourea
	Allylthiomocovina
	(2-Propenyl)thiourea
	Thiocynamine
	Tiosinamine
	NSC 1915
	Thiourea, N-2-propen-1-yl-
Inchi:	InChI=1S/C4H8N2S/c1-2-3-6-4(5)7/h2H,1,3H2,(H3,5,6,7)
InchiKey:	HTKFORQRBXIQHD-UHFFFAOYSA-N
Formula:	C4H8N2S
SMILES:	C=CCNC(=N)S
Mol. weight [g/mol]:	116.19
CAS:	109-57-9

Physical Properties

Property code	Value	Unit	Source
gf	393.02	kJ/mol	Joback Method
hf	289.82	kJ/mol	Joback Method
hvap	49.08	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	0.627		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
tb	484.97	K	Joback Method
tf	290.98	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.27	J/mol×K	484.97	Joback Method
cpg	42.12	J/mol×K	100.12	Joback Method
cpg	42.12	J/mol×K	100.12	Joback Method
cpg	42.12	J/mol×K	100.12	Joback Method
cpg	42.12	J/mol×K	100.12	Joback Method
cpg	42.12	J/mol×K	100.12	Joback Method
cpg	42.12	J/mol×K	100.12	Joback Method

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=C109579&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
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point