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

Physical Properties

Property code	Value	Unit	Source
hf	96.83	kJ/mol	Cheméo Relay (1.0)
hfus	19.74	kJ/mol	Joback Method
logp	0.006		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
tf	350.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.76	J/mol×K	480.34	Joback Method
cpg	195.06	J/mol×K	517.02	Joback Method
cpg	202.72	J/mol×K	553.71	Joback Method
cpg	209.80	J/mol×K	590.39	Joback Method
cpg	216.34	J/mol×K	627.08	Joback Method
cpg	222.39	J/mol×K	663.76	Joback Method
cpg	228.03	J/mol×K	700.45	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109579&Units=SI

Legend

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point