2(1H)-Pyrimidinethione, tetrahydro-

Other names:	Cyclic propylene thiourea
	Hexahydropyrimidine-2-thione
	N,N'-Trimethylenethiourea
	Tetrahydro-2(1H)-pyrimidinethione
	Tetrahydropyrimidine-2-thione
	Thiourea, N,N'-1,3-propanediyl-
	1,3-Propylenethiourea
	1,4,5,6-Tetrahydro-2-pyrimidinethiol
	2-Mercapto-1,4,5,6-tetrahydropyrimidine
	2-Mercapto-3,4,5,6-tetrahydropyrimidine
	2-Mercaptotetrahydropyrimidine
	3,4,5,6-Tetrahydro-2-pyrimidinethiol
	Perhydropyrimidine-2-thione
	3,4,5,6-Tetrahydro-2(1H)-pyrimidinethione
	NSC 21316
	3,4,5,6-tetrahydropyrimidine-2-thiol
Inchi:	InChI=1S/C4H8N2S/c7-4-5-2-1-3-6-4/h1-3H2,(H2,5,6,7)
InchiKey:	NVHNGVXBCWYLFA-UHFFFAOYSA-N
Formula:	C4H8N2S
SMILES:	S=C1NCCCN1
Mol. weight [g/mol]:	116.19
CAS:	2055-46-1

Physical Properties

Property code	Value	Unit	Source
gf	281.23	kJ/mol	Joback Method
hf	139.49	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	-0.146		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	6400.00	kPa	Joback Method
tb	484.88	K	Joback Method
tc	738.51	K	Joback Method
tf	420.19	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.33	J/mol×K	484.88	Joback Method
cpg	176.34	J/mol×K	527.15	Joback Method
cpg	186.63	J/mol×K	569.42	Joback Method
cpg	196.26	J/mol×K	611.69	Joback Method
cpg	205.24	J/mol×K	653.97	Joback Method
cpg	213.60	J/mol×K	696.24	Joback Method
cpg	221.38	J/mol×K	738.51	Joback Method

Sources

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=C2055461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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