THIOUREA, N-(HYDROXYMETHYL)-N'-METHYL-

Other names: Thiourea, N-(hydroxymethyl)-N'-methyl-
Urea, 1-(hydroxymethyl)-3-methyl-2-thio-
Gynaflex
N-(Hydroxymethyl)-N'-methylthiourea
1-(Hydroxymethyl)-3-methyl-2-thiourea
Noxyflex S
Noxythiolin
Noxythioline
Noxytioline

Inchi: InChI=1S/C3H8N2OS/c1-4-3(7)5-2-6/h6H,2H2,1H3,(H2,4,5,7)

InchiKey: JLMHZVYLAQPMOZ-UHFFFAOYSA-N

Formula: C3H8N2OS

SMILES: CNC(=S)NCO

Mol. weight [g/mol]: 120.18

Physical Properties

Property code	Value	Unit	Source
hfus	22.42	kJ/mol	Joback Method
ie	8.15	eV	Cheméo Relay (1.0)
logp	-0.970		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tf	382.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.06	J/mol×K	530.60	Joback Method
cpg	200.71	J/mol×K	563.13	Joback Method
cpg	206.93	J/mol×K	595.66	Joback Method
cpg	212.75	J/mol×K	628.19	Joback Method
cpg	218.21	J/mol×K	660.72	Joback Method
cpg	223.33	J/mol×K	693.25	Joback Method

cpg	228.15	J/mol×K	725.78	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=C15599390&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point