

Thiomorpholine

Other names:	Thiamorpholine Parathiazan Tetrahydro-1,4-thiazine 1,4-Thiazan 1-Thia-4-azacyclohexane 1,4-Thiazane 1,4-Thiazine, tetrahydro- thiazolidinane
Inchi:	InChI=1S/C4H9NS/c1-3-6-4-2-5-1/h5H,1-4H2
InchiKey:	BRNULMACUQOKMR-UHFFFAOYSA-N
Formula:	C4H9NS
SMILES:	C1CSCCN1
Mol. weight [g/mol]:	103.19
CAS:	123-90-0

Physical Properties

Property code	Value	Unit	Source
gf	142.53	kJ/mol	Joback Method
hf	31.84	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	37.81	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.323		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
rinpol	973.00		NIST Webbook
tb	411.52	K	Joback Method
tc	649.12	K	Joback Method
tf	334.94	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	140.63	J/mol×K	411.52	Joback Method
cpg	153.01	J/mol×K	451.12	Joback Method
cpg	164.70	J/mol×K	490.72	Joback Method
cpg	175.72	J/mol×K	530.32	Joback Method
cpg	186.08	J/mol×K	569.92	Joback Method
cpg	195.81	J/mol×K	609.52	Joback Method
cpg	204.92	J/mol×K	649.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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