Thioproperazine M (ring)

Inchi: InChI=1S/C14H14N2O2S2/c1-16(2)20(17,18)10-7-8-14-12(9-10)15-11-5-3-4-6-13(11)19-
InchiKey: KMMXCCWCGOUAGH-UHFFFAOYSA-N
Formula: C14H14N2O2S2
SMILES: CN(C)S(=O)(=O)c1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	113.30	kJ/mol	Joback Method
hf	-97.09	kJ/mol	Joback Method
hfus	45.74	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.145		Crippen Method
mcvol	214.140	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	3200.00		NIST Webbook
tb	751.76	K	Joback Method
tc	998.69	K	Joback Method
tf	623.15	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.32	J/mol×K	751.76	Joback Method
cpg	577.34	J/mol×K	792.91	Joback Method
cpg	590.14	J/mol×K	834.07	Joback Method
cpg	601.84	J/mol×K	875.22	Joback Method
cpg	612.53	J/mol×K	916.38	Joback Method
cpg	622.30	J/mol×K	957.53	Joback Method
cpg	631.27	J/mol×K	998.69	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=R212838&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume