Sulforidazine M (ring)

Inchi: InChI=1S/C13H11NO2S2/c1-18(15,16)9-6-7-13-11(8-9)14-10-4-2-3-5-12(10)17-13/h2-8,1
InchiKey: XMSALNTWEPZQLO-UHFFFAOYSA-N
Formula: C13H11NO2S2
SMILES: CS(=O)(=O)c1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-5.90	kJ/mol	Joback Method
hf	-143.98	kJ/mol	Joback Method
hfus	40.13	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.298		Crippen Method
mcvol	190.070	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	3180.00		NIST Webbook
rinpol	3180.00		NIST Webbook
tb	716.44	K	Joback Method
tc	973.30	K	Joback Method
tf	579.41	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.60	J/mol×K	716.44	Joback Method
cpg	486.05	J/mol×K	759.25	Joback Method
cpg	498.29	J/mol×K	802.06	Joback Method
cpg	509.43	J/mol×K	844.87	Joback Method
cpg	519.55	J/mol×K	887.68	Joback Method
cpg	528.74	J/mol×K	930.49	Joback Method
cpg	537.10	J/mol×K	973.30	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R212769&Units=SI

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