Periciazine M (ring)

Inchi: InChI=1S/C13H8N2S/c14-8-9-5-6-13-11(7-9)15-10-3-1-2-4-12(10)16-13/h1-7,15H
InchiKey: XZSIGWOVDPSPMG-UHFFFAOYSA-N
Formula: C13H8N2S
SMILES: N#Cc1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]: 224.28

Physical Properties

Property code	Value	Unit	Source
gf	595.82	kJ/mol	Joback Method
hf	474.25	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	74.17	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.766		Crippen Method
mcvol	163.360	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	2552.00		NIST Webbook
tb	770.74	K	Joback Method
tc	1051.16	K	Joback Method
tf	605.84	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.55	J/mol×K	770.74	Joback Method
cpg	413.37	J/mol×K	817.48	Joback Method
cpg	423.38	J/mol×K	864.21	Joback Method
cpg	432.71	J/mol×K	910.95	Joback Method
cpg	441.52	J/mol×K	957.69	Joback Method
cpg	449.96	J/mol×K	1004.42	Joback Method
cpg	458.18	J/mol×K	1051.16	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=R212556&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