3,7-Dimethylphenothiazine

Inchi: InChI=1S/C14H13NS/c1-9-3-5-11-13(7-9)16-14-8-10(2)4-6-12(14)15-11/h3-8,15H,1-2H3
InchiKey: SGMYETCUJUEWJU-UHFFFAOYSA-N
Formula: C14H13NS
SMILES: Cc1ccc2c(c1)Sc1cc(C)ccc1N2
Mol. weight [g/mol]: 227.32
CAS: 20751-71-7

Physical Properties

Property code	Value	Unit	Source
gf	461.43	kJ/mol	Joback Method
hf	277.26	kJ/mol	Joback Method
hfus	30.95	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.512		Crippen Method
mcvol	176.070	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	696.52	K	Joback Method
tc	961.85	K	Joback Method
tf	564.64	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.68	J/mol×K	696.52	Joback Method
cpg	453.31	J/mol×K	740.74	Joback Method
cpg	466.85	J/mol×K	784.96	Joback Method
cpg	479.43	J/mol×K	829.18	Joback Method
cpg	491.17	J/mol×K	873.41	Joback Method
cpg	502.19	J/mol×K	917.63	Joback Method
cpg	512.62	J/mol×K	961.85	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=C20751717&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume