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]: 227.33

Physical Properties

Property code	Value	Unit	Source
hf	195.91	kJ/mol	Cheméo Relay (1.0)
hfus	30.95	kJ/mol	Joback Method
ie	6.89	eV	Cheméo Relay (1.0)
log10ws	-6.17		Cheméo Relay (1.0)
logp	4.512		Crippen Method
mcvol	176.070	ml/mol	McGowan Method
tb	656.09	K	Cheméo Relay (1.0)
tf	491.68	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20751717&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point