Phenothiazine, 4-(trifluoromethyl)-

Inchi: InChI=1S/C13H8F3NS/c14-13(15,16)8-4-3-6-10-12(8)18-11-7-2-1-5-9(11)17-10/h1-7,17H
InchiKey: NSWKFLADKSTFDS-UHFFFAOYSA-N
Formula: C13H8F3NS
SMILES: FC(F)(F)c1cccc2c1Sc1ccccc1N2
Mol. weight [g/mol]: 267.27
CAS: 343-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-118.95	kJ/mol	Joback Method
hf	-287.71	kJ/mol	Joback Method
hfus	30.58	kJ/mol	Joback Method
hvap	59.94	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.914		Crippen Method
mcvol	167.290	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	663.24	K	Joback Method
tc	911.56	K	Joback Method
tf	545.04	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.52	J/mol×K	663.24	Joback Method
cpg	429.98	J/mol×K	704.63	Joback Method
cpg	441.33	J/mol×K	746.01	Joback Method
cpg	451.72	J/mol×K	787.40	Joback Method
cpg	461.29	J/mol×K	828.79	Joback Method
cpg	470.19	J/mol×K	870.18	Joback Method
cpg	478.56	J/mol×K	911.56	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=C343215&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume