10H-Phenothiazine, 2-(trifluoromethyl)-

Other names: Phenothiazine, 2-(trifluoromethyl)-
2-(Trifluoromethyl)phenothiazine
Trifluoromethylphenothiazine
Inchi: InChI=1S/C13H8F3NS/c14-13(15,16)8-5-6-12-10(7-8)17-9-3-1-2-4-11(9)18-12/h1-7,17H
InchiKey: RKGYJVASTMCSHZ-UHFFFAOYSA-N
Formula: C13H8F3NS
SMILES: FC(F)(F)c1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]: 267.27
CAS: 92-30-8

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
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
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

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=C92308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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