

10H-Phenothiazine, 3-methoxy-

Other names:	Phenothiazine, 3-methoxy- 3-Methoxyphenothiazine 10H-Dibenzo[b,E]-1,4-thiazine, 3-methoxy- 3-methoxy-10H-phenothiazine
Inchi:	InChI=1S/C13H11NOS/c1-15-9-6-7-11-13(8-9)16-12-5-3-2-4-10(12)14-11/h2-8,14H,1H3
InchiKey:	NKRGJNZQQYJCJHD-UHFFFAOYSA-N
Formula:	C13H11NOS
SMILES:	COc1ccc2c(c1)Sc1cccc1N2
Mol. weight [g/mol]:	229.30
CAS:	1771-19-3

Physical Properties

Property code	Value	Unit	Source
gf	357.64	kJ/mol	Joback Method
hf	177.15	kJ/mol	Joback Method
hfus	29.94	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.903		Crippen Method
mcvol	167.850	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	691.08	K	Joback Method
tc	957.09	K	Joback Method
tf	563.08	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.86	J/mol×K	691.08	Joback Method
cpg	427.69	J/mol×K	735.41	Joback Method
cpg	440.43	J/mol×K	779.75	Joback Method
cpg	452.19	J/mol×K	824.08	Joback Method
cpg	463.07	J/mol×K	868.42	Joback Method

cpg	473.17	J/mol×K	912.75	Joback Method
cpg	482.60	J/mol×K	957.09	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=C1771193&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

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