

10H-Phenothiazine, 2-(ethylthio)-

Other names:	2-(Ethylthio)phenothiazine Thiethylperazine M (ring)
Inchi:	InChI=1S/C14H13NS2/c1-2-16-10-7-8-14-12(9-10)15-11-5-3-4-6-13(11)17-14/h3-9,15H.2
InchiKey:	DMHPUUIDINBWB-N-UHFFFAOYSA-N
Formula:	C14H13NS2
SMILES:	CCSc1ccc2c(c1)Nc1cccc1S2
Mol. weight [g/mol]:	259.39
CAS:	46815-10-5

Physical Properties

Property code	Value	Unit	Source
gf	504.18	kJ/mol	Joback Method
hf	330.60	kJ/mol	Joback Method
hfus	35.47	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	5.007		Crippen Method
mcvol	192.420	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	2750.00		NIST Webbook
tb	760.32	K	Joback Method
tc	1040.84	K	Joback Method
tf	586.52	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.99	J/mol×K	760.32	Joback Method
cpg	503.13	J/mol×K	807.07	Joback Method
cpg	516.12	J/mol×K	853.83	Joback Method
cpg	528.09	J/mol×K	900.58	Joback Method
cpg	539.21	J/mol×K	947.33	Joback Method
cpg	549.60	J/mol×K	994.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C46815105&Units=SI
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

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

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