N,N-Dimethyl-1,2,3-trithian-5-amine

Other names:	Thiocyclam
	1,2,3-Trithian-5-amine, N,N-dimethyl-
	Evisekt
	Thiocyclam, methyl ester
Inchi:	InChI=1S/C5H11NS3/c1-6(2)5-3-7-9-8-4-5/h5H,3-4H2,1-2H3
InchiKey:	DNVLJEWNNDHELH-UHFFFAOYSA-N
Formula:	C5H11NS3
SMILES:	CN(C)C1CSSSC1
Mol. weight [g/mol]:	181.34
CAS:	31895-21-3

Physical Properties

Property code	Value	Unit	Source
gf	246.03	kJ/mol	Joback Method
hf	111.10	kJ/mol	Joback Method
hfus	14.53	kJ/mol	Joback Method
hvap	46.63	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.960		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	489.28	K	Joback Method
tc	744.48	K	Joback Method
tf	436.31	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	258.37	J/mol×K	489.28	Joback Method
cpg	273.47	J/mol×K	531.81	Joback Method
cpg	287.46	J/mol×K	574.35	Joback Method
cpg	300.42	J/mol×K	616.88	Joback Method
cpg	312.38	J/mol×K	659.42	Joback Method
cpg	323.42	J/mol×K	701.95	Joback Method
cpg	333.58	J/mol×K	744.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31895213&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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