2H-Thiopyran, tetrahydro-, 1-oxide

Other names:	Thiane 1-oxide
	Pentamethylene sulfoxide
	Tetrahydro-2H-thiopyran 1-oxide
	Tetrahydrothiopyran oxide
	Thiacyclohexane 1-oxide
	Thiane oxide
Inchi:	InChI=1S/C5H10OS/c6-7-4-2-1-3-5-7/h1-5H2
InchiKey:	NNLBRYQGMOYARS-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	O=S1CCCCC1
Mol. weight [g/mol]:	118.20
CAS:	4988-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-187.59	kJ/mol	Joback Method
hf	-274.22	kJ/mol	Joback Method
hfus	6.75	kJ/mol	Joback Method
hvap	39.18	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.919		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
tb	375.35	K	Joback Method
tc	583.29	K	Joback Method
tf	243.26	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.75	J/mol×K	375.35	Joback Method
cpg	166.27	J/mol×K	410.01	Joback Method
cpg	179.09	J/mol×K	444.66	Joback Method

cpg	191.22	J/mol×K	479.32	Joback Method
cpg	202.67	J/mol×K	513.98	Joback Method
cpg	213.47	J/mol×K	548.64	Joback Method
cpg	223.64	J/mol×K	583.29	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=C4988345&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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