Thietane, 1-oxide

Other names:	Trimethylene sulfoxide
	Thietane S-oxide
	1,3-Propanesulfone
	Thietane oxide
Inchi:	InChI=1S/C3H6OS/c4-5-2-1-3-5/h1-3H2
InchiKey:	GINSRDSEEGBTJO-UHFFFAOYSA-N
Formula:	C3H6OS
SMILES:	O=S1CCC1
Mol. weight [g/mol]:	90.14
CAS:	13153-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-180.23	kJ/mol	Joback Method
hf	-220.62	kJ/mol	Joback Method
hfus	5.77	kJ/mol	Joback Method
hvap	34.39	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	0.39		Crippen Method
logp	0.139		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
tb	321.05	K	Joback Method
tc	512.49	K	Joback Method
tf	227.76	K	Joback Method
vc	0.235	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.14	J/mol×K	321.05	Joback Method
cpg	98.97	J/mol×K	352.96	Joback Method
cpg	107.28	J/mol×K	384.86	Joback Method

cpg	115.09	J/mol×K	416.77	Joback Method
cpg	122.43	J/mol×K	448.68	Joback Method
cpg	129.32	J/mol×K	480.59	Joback Method
cpg	135.77	J/mol×K	512.49	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=C13153112&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
ie:	Ionization energy
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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