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	8.96	eV	NIST Webbook
ie	8.50	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: 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=C13153112&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
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