

Thiirane, (methoxymethyl)-

Other names:	2,3-Epithiopropyl methyl ether Ether, 2,3-epithiopropyl methyl (Methoxymethyl)thiirane 2-(Methoxymethyl)thiirane Thiirane, 2-(methoxymethyl)- 2,3-Epithiopropyl methoxy ether
Inchi:	InChI=1S/C4H8OS/c1-5-2-4-3-6-4/h4H,2-3H2,1H3
InchiKey:	SVUNGRWSYPGFNP-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	COCC1CS1
Mol. weight [g/mol]:	104.17
CAS:	19858-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-21.59	kJ/mol	Joback Method
hf	-140.05	kJ/mol	Joback Method
hfus	9.10	kJ/mol	Joback Method
hvap	32.63	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
log10ws	-0.47		Crippen Method
logp	0.748		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
tb	367.91	K	Joback Method
tc	566.14	K	Joback Method
tf	258.46	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	136.03	J/mol×K	367.91	Joback Method
cpg	145.23	J/mol×K	400.95	Joback Method
cpg	153.96	J/mol×K	433.99	Joback Method
cpg	162.24	J/mol×K	467.03	Joback Method
cpg	170.10	J/mol×K	500.07	Joback Method
cpg	177.55	J/mol×K	533.11	Joback Method
cpg	184.60	J/mol×K	566.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19858141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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