

Thiophene, tetrahydro-, 1-oxide

Other names:	Tetrahydrothiophene oxide
	Tetrahydrothiophene 1-oxide
	Tetramethylene sulfoxide
	Thiophane monoxide
	Thiophane oxide
	Thiophane 1-oxide
	Thiophene-1-oxide, tetrahydro-
	Thiolane 1-oxide
	Tetramethylene sulphoxide
	Tetramethylene sulfoxide
	NSC 65433
	Tetrahydrothiophene S-oxide
Inchi:	InChI=1S/C4H8OS/c5-6-3-1-2-4-6/h1-4H2
InchiKey:	ISXOBTBCNRIIQO-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	O=S1CCCC1
Mol. weight [g/mol]:	104.17
CAS:	1600-44-8

Physical Properties

Property code	Value	Unit	Source
ea	0.02 ± 0.00	eV	NIST Webbook
gf	-183.91	kJ/mol	Joback Method
hf	-247.42	kJ/mol	Joback Method
hfus	6.26	kJ/mol	Joback Method
hvap	36.78	kJ/mol	Joback Method
ie	9.07 ± 0.05	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
log10ws	-0.03		Crippen Method
logp	0.529		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	5687.39	kPa	Joback Method
tb	348.20	K	Joback Method
tc	548.28	K	Joback Method
tf	235.51	K	Joback Method

vc	0.283	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.66	J/mol×K	348.20	Joback Method
cpg	130.83	J/mol×K	381.55	Joback Method
cpg	141.39	J/mol×K	414.89	Joback Method
cpg	151.35	J/mol×K	448.24	Joback Method
cpg	160.76	J/mol×K	481.59	Joback Method
cpg	169.61	J/mol×K	514.94	Joback Method
cpg	177.95	J/mol×K	548.28	Joback Method
hfust	0.51	kJ/mol	231.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1600448&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

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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