1,3-Oxathiolane

Other names: 1,3-Oxathiole, dihydro-
1,3-Oxothiolane
Inchi: InChI=1S/C3H6OS/c1-2-5-3-4-1/h1-3H2
InchiKey: WJJSZTJGFCFNKI-UHFFFAOYSA-N
Formula: C3H6OS
SMILES: C1CSCO1
Mol. weight [g/mol]: 90.14
CAS: 2094-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-27.62	kJ/mol	Joback Method
hf	-111.17	kJ/mol	Joback Method
hfus	8.03	kJ/mol	Joback Method
hvap	33.16	kJ/mol	Joback Method
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-0.44		Crippen Method
logp	0.707		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	5845.00	kPa	Joback Method
rinpol	806.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	788.00		NIST Webbook
tb	362.77	K	Joback Method
tc	582.76	K	Joback Method
tf	248.73	K	Joback Method
vc	0.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.55	J/mol×K	362.77	Joback Method
cpg	109.69	J/mol×K	399.44	Joback Method
cpg	118.26	J/mol×K	436.10	Joback Method
cpg	126.27	J/mol×K	472.77	Joback Method
cpg	133.75	J/mol×K	509.43	Joback Method
cpg	140.73	J/mol×K	546.10	Joback Method
cpg	147.24	J/mol×K	582.76	Joback Method

Sources

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=C2094975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume