1,3-Oxathiolane, 2-methyl-2-isopropyl-

Other names: 2-Methyl-2-propan-2-yl-1,3-oxathiolane
Inchi: InChI=1S/C7H14OS/c1-6(2)7(3)8-4-5-9-7/h6H,4-5H2,1-3H3
InchiKey: RGMFYYDYJLBLOW-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CC(C)C1(C)OCCS1
Mol. weight [g/mol]: 146.25
CAS: 16047-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-9.58	kJ/mol	Joback Method
hf	-204.11	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.122		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
tb	449.42	K	Joback Method
tc	674.46	K	Joback Method
tf	298.47	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.38	J/mol×K	449.42	Joback Method
cpg	268.10	J/mol×K	486.93	Joback Method
cpg	282.63	J/mol×K	524.43	Joback Method
cpg	296.07	J/mol×K	561.94	Joback Method
cpg	308.58	J/mol×K	599.45	Joback Method
cpg	320.27	J/mol×K	636.95	Joback Method

cpg	331.28	J/mol×K	674.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16047986&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
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
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