2-Isopropyl-1,3-oxothiolane

Inchi: InChI=1S/C6H12OS/c1-5(2)6-7-3-4-8-6/h5-6H,3-4H2,1-2H3
InchiKey: JTGZVABCBHZNLP-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC(C)C1OCCS1
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-12.51	kJ/mol	Joback Method
hf	-198.71	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	39.14	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.732		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1000.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	967.00		NIST Webbook
tb	426.30	K	Joback Method
tc	644.38	K	Joback Method
tf	263.30	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.66	J/mol×K	426.30	Joback Method
cpg	224.92	J/mol×K	462.65	Joback Method
cpg	238.39	J/mol×K	498.99	Joback Method

cpg	251.09	J/mol×K	535.34	Joback Method
cpg	263.06	J/mol×K	571.68	Joback Method
cpg	274.32	J/mol×K	608.03	Joback Method
cpg	284.90	J/mol×K	644.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78862&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