2-Isobutyl-1,3-oxothiolane

Inchi: InChI=1S/C7H14OS/c1-6(2)5-7-8-3-4-9-7/h6-7H,3-5H2,1-2H3
InchiKey: FYGCGLKHZOKOQI-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CC(C)CC1OCCS1
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	-4.09	kJ/mol	Joback Method
hf	-219.35	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	41.37	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.122		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1086.00		NIST Webbook
tb	449.18	K	Joback Method
tc	664.36	K	Joback Method
tf	274.57	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.59	J/mol×K	449.18	Joback Method
cpg	267.04	J/mol×K	485.04	Joback Method
cpg	281.63	J/mol×K	520.91	Joback Method
cpg	295.41	J/mol×K	556.77	Joback Method

cpg	308.39	J/mol×K	592.64	Joback Method
cpg	320.62	J/mol×K	628.50	Joback Method
cpg	332.12	J/mol×K	664.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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