Beta-isopropyl-beta-propiolactone

Inchi: InChI=1S/C6H10O2/c1-4(2)5-3-8-6(5)7/h4-5H,3H2,1-2H3
InchiKey: JFLMBMOAMWVCRC-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CC(C)C1COC1=O
Mol. weight [g/mol]: 114.14
CAS: 10359-02-1

Physical Properties

Property code	Value	Unit	Source
chl	-3368.00 ± 3.30	kJ/mol	NIST Webbook
gf	-162.86	kJ/mol	Joback Method
hf	-375.51	kJ/mol	Joback Method
hfl	-422.20 ± 3.30	kJ/mol	NIST Webbook
hfus	11.30	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	0.815		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	442.02	K	Joback Method
tc	655.52	K	Joback Method
tf	251.59	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.46	J/mol×K	442.02	Joback Method
cpg	206.93	J/mol×K	477.60	Joback Method
cpg	218.87	J/mol×K	513.19	Joback Method
cpg	230.28	J/mol×K	548.77	Joback Method
cpg	241.16	J/mol×K	584.36	Joback Method
cpg	251.50	J/mol×K	619.94	Joback Method
cpg	261.33	J/mol×K	655.52	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=C10359021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume