Beta-propyl-beta-propiolactone

Inchi: InChI=1S/C6H10O2/c1-2-3-5-4-8-6(5)7/h5H,2-4H2,1H3
InchiKey: RDILZTZKTCONPZ-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CCCC1COC1=O
Mol. weight [g/mol]: 114.14
CAS: 15964-17-7

Physical Properties

Property code	Value	Unit	Source
chl	-3337.60 ± 1.60	kJ/mol	NIST Webbook
gf	-160.42	kJ/mol	Joback Method
hf	-370.23	kJ/mol	Joback Method
hfl	-452.60 ± 1.60	kJ/mol	NIST Webbook
hfus	14.82	kJ/mol	Joback Method
hvap	37.79	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.959		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	442.46	K	Joback Method
tc	650.91	K	Joback Method
tf	266.59	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.35	J/mol×K	442.46	Joback Method
cpg	206.44	J/mol×K	477.20	Joback Method
cpg	218.02	J/mol×K	511.94	Joback Method
cpg	229.11	J/mol×K	546.68	Joback Method
cpg	239.70	J/mol×K	581.43	Joback Method
cpg	249.80	J/mol×K	616.17	Joback Method
cpg	259.40	J/mol×K	650.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15964177&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

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