dihydro-5-isopropyl-3(2H)-furanone

Inchi: InChI=1S/C7H12O2/c1-5(2)6-3-4-7(8)9-6/h5-6H,3-4H2,1-2H3
InchiKey: XTFLBVQDKFPSCS-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CC(C)C1CCC(=O)O1
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	-166.54	kJ/mol	Joback Method
hf	-402.31	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	39.80	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.348		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook
tb	469.17	K	Joback Method
tc	688.18	K	Joback Method
tf	259.34	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.44	J/mol×K	469.17	Joback Method
cpg	249.18	J/mol×K	505.67	Joback Method
cpg	263.26	J/mol×K	542.17	Joback Method
cpg	276.68	J/mol×K	578.68	Joback Method
cpg	289.44	J/mol×K	615.18	Joback Method
cpg	301.53	J/mol×K	651.68	Joback Method
cpg	312.96	J/mol×K	688.18	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=R321303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume