2(5H)-Furanone, 5-(1-methylethyl)-

Other names: 5-Isopropyl-5H-furan-2-one
Inchi: InChI=1S/C7H10O2/c1-5(2)6-3-4-7(8)9-6/h3-6H,1-2H3
InchiKey: LWFKYUIZWLTJCA-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC(C)C1C=CC(=O)O1
Mol. weight [g/mol]: 126.15
CAS: 56767-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-136.58	kJ/mol	Joback Method
hf	-344.53	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	40.09	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.124		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1311.00		NIST Webbook
tb	468.33	K	Joback Method
tc	689.64	K	Joback Method
tf	260.10	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.87	J/mol×K	468.33	Joback Method
cpg	232.27	J/mol×K	505.22	Joback Method
cpg	245.06	J/mol×K	542.10	Joback Method
cpg	257.22	J/mol×K	578.99	Joback Method
cpg	268.77	J/mol×K	615.87	Joback Method
cpg	279.69	J/mol×K	652.76	Joback Method
cpg	289.99	J/mol×K	689.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56767192&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

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