2,2-Dimethyl-3(2H)-furanone

Inchi: InChI=1S/C6H8O2/c1-6(2)5(7)3-4-8-6/h3-4H,1-2H3
InchiKey: HVNICCSXGONRCB-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1(C)OC=CC1=O
Mol. weight [g/mol]: 112.13
CAS: 35298-48-7

Physical Properties

Property code	Value	Unit	Source
gf	-148.05	kJ/mol	Joback Method
hf	-303.37	kJ/mol	Joback Method
hfus	7.64	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	446.13	K	Joback Method
tc	675.56	K	Joback Method
tf	287.73	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.23	J/mol×K	446.13	Joback Method
cpg	191.02	J/mol×K	484.37	Joback Method
cpg	201.97	J/mol×K	522.61	Joback Method
cpg	212.19	J/mol×K	560.84	Joback Method
cpg	221.76	J/mol×K	599.08	Joback Method
cpg	230.78	J/mol×K	637.32	Joback Method
cpg	239.35	J/mol×K	675.56	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=C35298487&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume