2-methyl-3(2H)-furanone

Inchi: InChI=1S/C5H6O2/c1-4-5(6)2-3-7-4/h2-4H,1H3
InchiKey: FAYUQJQOHOTTKW-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: CC1OC=CC1=O
Mol. weight [g/mol]: 98.10

Physical Properties

Property code	Value	Unit	Source
gf	-150.98	kJ/mol	Joback Method
hf	-297.97	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	36.03	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.488		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	814.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1396.00		NIST Webbook
tb	423.01	K	Joback Method
tc	645.30	K	Joback Method
tf	252.56	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.46	J/mol×K	423.01	Joback Method
cpg	150.58	J/mol×K	460.06	Joback Method
cpg	160.30	J/mol×K	497.11	Joback Method
cpg	169.61	J/mol×K	534.16	Joback Method
cpg	178.50	J/mol×K	571.20	Joback Method

cpg	186.96	J/mol×K	608.25	Joback Method
cpg	194.99	J/mol×K	645.30	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=R237788&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume