

3(2H)-Furanone, dihydro-5-methyl-

Other names:	5-Methyldihydro-3(2H)-furanone 3(2H)-Furanone, 4,5-dihydro-5-methyl
Inchi:	InChI=1S/C5H8O2/c1-4-2-5(6)3-7-4/h4H,2-3H2,1H3
InchiKey:	YJZXJDJWRQIWDL-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1CC(=O)CO1
Mol. weight [g/mol]:	100.12
CAS:	34003-72-0

Physical Properties

Property code	Value	Unit	Source
gf	-180.94	kJ/mol	Joback Method
hf	-355.75	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	35.74	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.364		Crippen Method
mvol	77.890	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
rinpol	808.00		NIST Webbook
rinpol	822.00		NIST Webbook
tb	423.85	K	Joback Method
tc	643.76	K	Joback Method
tf	251.80	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.05	J/molxK	423.85	Joback Method
cpg	165.60	J/molxK	460.50	Joback Method
cpg	176.71	J/molxK	497.15	Joback Method
cpg	187.37	J/molxK	533.80	Joback Method
cpg	197.57	J/molxK	570.45	Joback Method

cpg	207.30	J/mol×K	607.10	Joback Method
cpg	216.54	J/mol×K	643.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C34003720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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

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