

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

Other names:	Dihydro-3,5-dimethyl-2(3H)-furanone 2-Methyl-4-pentanolide
Inchi:	InChI=1S/C6H10O2/c1-4-3-5(2)8-6(4)7/h4-5H,3H2,1-2H3
InchiKey:	IYJMJJJBGWGVKX-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC1CC(C)C(=O)O1
Mol. weight [g/mol]:	114.14
CAS:	5145-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-180.23	kJ/mol	Joback Method
hf	-396.73	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	37.66	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.958		Crippen Method
mvol	91.980	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	442.06	K	Joback Method
tc	658.70	K	Joback Method
tf	258.83	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.95	J/mol×K	442.06	Joback Method
cpg	207.25	J/mol×K	478.17	Joback Method
cpg	220.06	J/mol×K	514.27	Joback Method
cpg	232.37	J/mol×K	550.38	Joback Method
cpg	244.15	J/mol×K	586.49	Joback Method
cpg	255.40	J/mol×K	622.59	Joback Method
cpg	266.11	J/mol×K	658.70	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=C5145017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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