Dihydro-3-methylene-5-methyl-2-furanone

Other names:	2(3H)-Furanone, dihydro-5-methyl-3-methylene- 5-Methyl-3-methylenedihydrofuran-2(3H)-one
Inchi:	InChI=1S/C6H8O2/c1-4-3-5(2)8-6(4)7/h5H,1,3H2,2H3
InchiKey:	KYLUHLJIAMFYKW-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	C=C1CC(C)OC1=O
Mol. weight [g/mol]:	112.13
CAS:	62873-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-119.44	kJ/mol	Joback Method
hf	-292.15	kJ/mol	Joback Method
hfus	11.56	kJ/mol	Joback Method
hvap	38.12	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	1074.50		NIST Webbook
rinpol	1074.50		NIST Webbook
tb	445.89	K	Joback Method
tc	664.94	K	Joback Method
tf	276.75	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.43	J/mol×K	445.89	Joback Method
cpg	189.73	J/mol×K	482.40	Joback Method
cpg	200.63	J/mol×K	518.91	Joback Method
cpg	211.10	J/mol×K	555.41	Joback Method
cpg	221.13	J/mol×K	591.92	Joback Method

cpg	230.71	J/mol×K	628.43	Joback Method
cpg	239.82	J/mol×K	664.94	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=C62873169&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

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