

2(3H)-Furanone, 4,5-dihydro-4-(2-methyl-3-methylenebut-4-yl)-

Other names:	4,5-Dihydro-4-(2-methyl-3-methylenebut-4-yl)-2(3H)-furanone
Inchi:	InChI=1S/C10H16O2/c1-7(2)8(3)4-9-5-10(11)12-6-9/h7,9H,3-6H2,1-2H3
InchiKey:	MEEDQJHQLVRLMF-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	<chem>C=C(CC1COC(=O)C1)C(C)C</chem>
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	-61.99	kJ/mol	Joback Method
hf	-348.59	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.152		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1195.00		NIST Webbook
rinpol	1195.00		NIST Webbook
tb	534.37	K	Joback Method
tc	751.80	K	Joback Method
tf	277.43	K	Joback Method
vc	0.540	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.03	J/mol×K	534.37	Joback Method
cpg	368.37	J/mol×K	570.61	Joback Method
cpg	384.82	J/mol×K	606.85	Joback Method
cpg	400.38	J/mol×K	643.08	Joback Method
cpg	415.06	J/mol×K	679.32	Joback Method
cpg	428.89	J/mol×K	715.56	Joback Method
cpg	441.86	J/mol×K	751.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U153914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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