

2(3H)-FURANONE, 4,5-DIHYDRO-4-(2-METHYL-3-METHYLENEBUT-4-

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:	C=C(CC1COC(=O)C1)C(C)C
Mol. weight [g/mol]:	168.24

Physical Properties

Property code	Value	Unit	Source
hfus	16.97	kJ/mol	Joback Method
logp	2.152		Crippen Method
mcpvol	144.040	ml/mol	McGowan Method
rinpol	1195.00		NIST Webbook

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U153914&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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