

3-Hydroxycarbofuran

Other names:

3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-, 7-(methylcarbamate)
Carbamic acid, methyl-, 2,3-dihydro-3-hydroxy-2,2-dimethyl-7-benzofuranyl ester
Carbamic acid, methyl-, 2,3-dihydro-2,2-dimethyl-3-hydroxy-7-benzofuranyl ester
Carbofuran 3-oh
Carbofuran, 3-hydroxy

Inchi: InChI=1S/C12H15NO4/c1-12(2)10(14)7-5-4-6-8(9(7)17-12)16-11(15)13-3/h4-6,10,14H,1-**InchiKey:** RHSUJRQZTQNSLL-UHFFFAOYSA-N**Formula:** C12H15NO4**SMILES:** CNC(=O)Oc1cccc2c1OC(C)(C)C2O**Mol. weight [g/mol]:** 237.25**CAS:** 16655-82-6

Physical Properties

Property code	Value	Unit	Source
gf	-176.61	kJ/mol	Joback Method
hf	-485.28	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	81.14	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.609		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	758.50	K	Joback Method
tc	970.66	K	Joback Method
tf	526.27	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.39	J/molxK	758.50	Joback Method
cpg	522.63	J/molxK	793.86	Joback Method
cpg	534.49	J/molxK	829.22	Joback Method
cpg	546.09	J/molxK	864.58	Joback Method

cpg	557.54	J/mol×K	899.94	Joback Method
cpg	568.96	J/mol×K	935.30	Joback Method
cpg	580.46	J/mol×K	970.66	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=C16655826&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
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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