Carbofuran

Other names:

(2,2-dimethyl-3H-1-benzofuran-7-yl) N-methylcarbamate
2,2-Dimethyl-2,2-dihydrobenzofuranyl-7 N-methylcarbamate
2,2-Dimethyl-2,3-dihydro-7-benzofuranyl N-methylcarbamate
2,2-Dimethyl-2,3-dihydrobenzoduranyl-7-N-methylcarbamate
2,2-Dimethyl-7-Coumaranyl N-methylcarbamate
2,3-Dihydro-2,2-dimethyl-7-benzofuranol methylcarbamate
2,3-Dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate
2,3-Dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate
2,3-Dihydro-2,2-dimethylbenzofuranyl-7-N-methylcarbamate
7-Benzofurano, 2,3-dihydro-2,2-dimethyl, methylcarbamate
7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-, 7-(N-methylcarbamate)
7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-, methylcarbamate
BAY 70143
BAY 78537
Benzofuran-7-ol, 2,3-dihydro, 2,2-dimethyl, N-methylcarbamate
C2292-59a
Carbamic acid, methyl-, 2,2-dimethyl-2,3-dihydro-7-benzofuranyl ester
Carbamic acid, methyl-, 2,2-dimethyl-2,3-dihydrobenzofuran-7-yl ester
Carbamic acid, methyl-, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester
Carbodan
Carbofurane
Chinufur
Crisfuran
Curaterr
D 1221
ENT 27,164
FMC 10242
Furacarb
Furadan
Furadan 3G
Furadan 4F
Furadan 75 WP
Furadan G
Furadane
Karbofuranu
Me f248
Methyl carbamic acid 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester
NA 2757
NIA 10242
Niagara 10242

Niagara nia-10242
OMS 864
Rampart
Yaltox

Inchi: InChI=1S/C12H15NO3/c1-12(2)7-8-5-4-6-9(10(8)16-12)15-11(14)13-3/h4-6H,7H2,1-3H3,

InchiKey: DUEPRVBVGDRKAG-UHFFFAOYSA-N

Formula: C12H15NO3

SMILES: CNC(=O)Oc1cccc2c1OC(C)(C)C2

Mol. weight [g/mol]: 221.25

CAS: 1563-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-32.08	kJ/mol	Joback Method
hf	-312.71	kJ/mol	Joback Method
hfus	27.80	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
log10ws	-2.80		Estimated Solubility Method
log10ws	-2.50		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.38		Aqueous Solubility Prediction Method
logp	2.118		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	670.99	K	Joback Method
tc	898.37	K	Joback Method
tf	424.40	K	Aqueous Solubility Prediction Method

tf	426.38 ± 0.20	K	NIST Webbook
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.28	J/mol×K	860.47	Joback Method
cpg	455.84	J/mol×K	670.99	Joback Method
cpg	469.83	J/mol×K	708.89	Joback Method
cpg	483.13	J/mol×K	746.78	Joback Method
cpg	495.87	J/mol×K	784.68	Joback Method
cpg	508.21	J/mol×K	822.58	Joback Method
cpg	532.23	J/mol×K	898.37	Joback Method
hfust	30.33	kJ/mol	426.20	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563662&Units=SI

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

hfust: Enthalpy of fusion at a given temperature

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