

Benzofuran, 2,3-dihydro-2,2,4,6-tetramethyl-

Other names:	2,3-Dihydro-2,2,4,6-tetramethylbenzofuran
Inchi:	InChI=1S/C12H16O/c1-8-5-9(2)10-7-12(3,4)13-11(10)6-8/h5-6H,7H2,1-4H3
InchiKey:	NKEPZWFYNPDTND-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	<chem>Cc1cc(C)c2c(c1)OC(C)(C)C2</chem>
Mol. weight [g/mol]:	176.25
CAS:	3698-49-5

Physical Properties

Property code	Value	Unit	Source
gf	102.82	kJ/mol	Joback Method
hf	-132.85	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	49.84	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.017		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	549.51	K	Joback Method
tc	775.17	K	Joback Method
tf	357.39	K	Joback Method
vc	0.576	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.27	J/molxK	549.51	Joback Method
cpg	379.11	J/molxK	587.12	Joback Method
cpg	393.91	J/molxK	624.73	Joback Method
cpg	407.82	J/molxK	662.34	Joback Method
cpg	420.98	J/molxK	699.95	Joback Method
cpg	433.55	J/molxK	737.56	Joback Method
cpg	445.69	J/molxK	775.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3698495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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