

Benzofuran, 2,3-dihydro-2,2,7-trimethyl-

Inchi:	InChI=1S/C11H14O/c1-8-5-4-6-9-7-11(2,3)12-10(8)9/h4-6H,7H2,1-3H3
InchiKey:	OWRJMGJBGSBJHE-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	Cc1cccc2c1OC(C)(C)C2
Mol. weight [g/mol]:	162.23
CAS:	30590-60-4

Physical Properties

Property code	Value	Unit	Source
gf	104.03	kJ/mol	Joback Method
hf	-100.74	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hvap	46.95	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.709		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	521.65	K	Joback Method
tc	750.34	K	Joback Method
tf	333.60	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.27	J/molxK	521.65	Joback Method
cpg	332.75	J/molxK	559.77	Joback Method
cpg	347.08	J/molxK	597.88	Joback Method
cpg	360.41	J/molxK	636.00	Joback Method
cpg	372.91	J/molxK	674.11	Joback Method
cpg	384.74	J/molxK	712.23	Joback Method
cpg	396.05	J/molxK	750.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30590604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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
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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