7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-

Other names:	Carbofuran phenol
	Nia 10272
	2,3-Dihydro-2,2-dimethyl-7-benzofuranol
	2,3-Dihydro-2,2-dimethyl-7-hydroxybenzofuran
	Carbofuran 7-phenol
	Carbofuran-7-ol
	2,3-dihydro-2,2-dimethylbenzofuran-7-ol
Inchi:	InChI=1S/C10H12O2/c1-10(2)6-7-4-3-5-8(11)9(7)12-10/h3-5,11H,6H2,1-2H3
InchiKey:	WJGPNUBJBMCRQH-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC1(C)Cc2cccc(O)c2O1
Mol. weight [g/mol]:	164.20
CAS:	1563-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-49.38	kJ/mol	Joback Method
hf	-245.94	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.106		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	574.41	K	Joback Method
tc	818.22	K	Joback Method
tf	421.53	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.41	J/mol×K	574.41	Joback Method
cpg	336.36	J/mol×K	615.05	Joback Method
cpg	348.27	J/mol×K	655.68	Joback Method
cpg	359.38	J/mol×K	696.32	Joback Method
cpg	369.96	J/mol×K	736.95	Joback Method
cpg	380.24	J/mol×K	777.59	Joback Method
cpg	390.50	J/mol×K	818.22	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=C1563388&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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