3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-

Other names:	3-Hydroxycarbofuran phenol
	Carbofuran-3-hydroxy-7-phenol
	Carbofuran 7-phenol 3-oh
	2,2-Dimethyl-2,3-dihydro-1-benzofuran-3,7-diol
	2,2-Dimethyl-3,7-dihydroxy-2,3-dihydrobenzofuran
	3-Hydroxycarbofuran-7-ol
Inchi:	InChI=1S/C10H12O3/c1-10(2)9(12)6-4-3-5-7(11)8(6)13-10/h3-5,9,11-12H,1-2H3
InchiKey:	CNFFSKAZCVPTPA-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CC1(C)Oc2c(O)cccc2C1O
Mol. weight [g/mol]:	180.20
CAS:	17781-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-193.91	kJ/mol	Joback Method
hf	-418.51	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.597		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	661.92	K	Joback Method
tc	885.04	K	Joback Method
tf	383.94 ± 0.20	K	NIST Webbook
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.83	J/mol×K	661.92	Joback Method
cpg	382.53	J/mol×K	699.11	Joback Method
cpg	392.75	J/mol×K	736.29	Joback Method

cpg	402.68	J/mol×K	773.48	Joback Method
cpg	412.52	J/mol×K	810.67	Joback Method
cpg	422.45	J/mol×K	847.85	Joback Method
cpg	432.65	J/mol×K	885.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17781156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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