3(2H)-Benzofuranone, 7-hydroxy-2,2-dimethyl-

Other names:	3-Ketocarbofuran phenol
	Carbofuran 3-keto 7-phenol
	7-Hydroxy-2,2-dimethyl-1-benzofuran-3(2H)-one
	2,3-Dihydro-7-hydroxy-2,2-dimethyl-3-ketobenzofuran
	3-Ketocarbofuran-7-ol
Inchi:	InChI=1S/C10H10O3/c1-10(2)9(12)6-4-3-5-7(11)8(6)13-10/h3-5,11H,1-2H3
InchiKey:	XLZCZWCXCBPEJR-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CC1(C)Oc2c(O)cccc2C1=O
Mol. weight [g/mol]:	178.18
CAS:	17781-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-171.97	kJ/mol	Joback Method
hf	-383.64	kJ/mol	Joback Method
hfus	20.42	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.746		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
tb	642.23	K	Joback Method
tc	899.29	K	Joback Method
tf	489.75	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.48	J/mol×K	642.23	Joback Method
cpg	355.69	J/mol×K	685.07	Joback Method
cpg	367.26	J/mol×K	727.92	Joback Method
cpg	378.45	J/mol×K	770.76	Joback Method

cpg	389.48	J/mol×K	813.61	Joback Method
cpg	400.62	J/mol×K	856.45	Joback Method
cpg	412.10	J/mol×K	899.29	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17781167&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
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