

Benzophenone, 4'-chloro-2,4-dihydroxy-

Inchi:	InChI=1S/C13H9ClO3/c14-9-3-1-8(2-4-9)13(17)11-6-5-10(15)7-12(11)16/h1-7,15-16H
InchiKey:	OKCRKLJFFOULPM-UHFFFAOYSA-N
Formula:	C13H9ClO3
SMILES:	O=C(c1ccc(Cl)cc1)c1ccc(O)cc1O
Mol. weight [g/mol]:	248.66
CAS:	18239-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-176.32	kJ/mol	Joback Method
hf	-333.00	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	86.91	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.982		Crippen Method
mcvol	172.060	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
tb	807.72	K	Joback Method
tc	1075.95	K	Joback Method
tf	604.92	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.87	J/mol×K	807.72	Joback Method
cpg	499.37	J/mol×K	1031.24	Joback Method
cpg	488.97	J/mol×K	986.54	Joback Method
cpg	478.95	J/mol×K	941.83	Joback Method
cpg	469.08	J/mol×K	897.13	Joback Method
cpg	459.13	J/mol×K	852.42	Joback Method
cpg	510.40	J/mol×K	1075.95	Joback Method
dvisc	0.0000007	Pa×s	807.72	Joback Method
dvisc	0.0000010	Pa×s	773.92	Joback Method

dvisc	0.0000015	Pa×s	740.12	Joback Method
dvisc	0.0000024	Pa×s	706.32	Joback Method
dvisc	0.0000040	Pa×s	672.52	Joback Method
dvisc	0.0000069	Pa×s	638.72	Joback Method
dvisc	0.0000127	Pa×s	604.92	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=C18239106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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