

Benzophenone, 3,5-dichloro-2-hydroxy-

Inchi:	InChI=1S/C13H8Cl2O2/c14-9-6-10(13(17)11(15)7-9)12(16)8-4-2-1-3-5-8/h1-7,17H
InchiKey:	KQEKLTCGLCEO FY-UHFFFAOYSA-N
Formula:	C13H8Cl2O2
SMILES:	O=C(c1ccccc1)c1cc(Cl)cc(Cl)c1O
Mol. weight [g/mol]:	267.11
CAS:	7396-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-43.26	kJ/mol	Joback Method
hf	-182.90	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.930		Crippen Method
mcvol	178.430	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	769.51	K	Joback Method
tc	1034.87	K	Joback Method
tf	535.64	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.78	J/molxK	769.51	Joback Method
cpg	438.05	J/molxK	813.74	Joback Method
cpg	447.57	J/molxK	857.96	Joback Method
cpg	456.49	J/molxK	902.19	Joback Method
cpg	464.97	J/molxK	946.42	Joback Method
cpg	473.15	J/molxK	990.64	Joback Method
cpg	481.19	J/molxK	1034.87	Joback Method
dvisc	0.0001714	Paxs	535.64	Joback Method
dvisc	0.0000957	Paxs	574.62	Joback Method

dvisc	0.0000576	Paxs	613.60	Joback Method
dvisc	0.0000368	Paxs	652.58	Joback Method
dvisc	0.0000247	Paxs	691.55	Joback Method
dvisc	0.0000173	Paxs	730.53	Joback Method
dvisc	0.0000126	Paxs	769.51	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=C7396921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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