

3',4'-Dichloro-2-hydroxy-5-methylbenzophenone

Inchi:	InChI=1S/C14H10Cl2O2/c1-8-2-5-13(17)10(6-8)14(18)9-3-4-11(15)12(16)7-9/h2-7,17H,1
InchiKey:	POGCHIPMLALUQZ-UHFFFAOYSA-N
Formula:	C14H10Cl2O2
SMILES:	<chem>Cc1ccc(O)c(C(=O)c2ccc(Cl)c(Cl)c2)c1</chem>
Mol. weight [g/mol]:	281.13
CAS:	92153-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-44.47	kJ/mol	Joback Method
hf	-215.01	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.238		Crippen Method
mcvol	192.520	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	797.37	K	Joback Method
tc	1057.37	K	Joback Method
tf	559.43	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.50	J/molxK	797.37	Joback Method
cpg	488.39	J/molxK	840.70	Joback Method
cpg	498.58	J/molxK	884.04	Joback Method
cpg	508.20	J/molxK	927.37	Joback Method
cpg	517.38	J/molxK	970.70	Joback Method
cpg	526.26	J/molxK	1014.04	Joback Method
cpg	534.98	J/molxK	1057.37	Joback Method
dvisc	0.0001217	Paxs	559.43	Joback Method
dvisc	0.0000703	Paxs	599.09	Joback Method

dvisc	0.0000434	Paxs	638.74	Joback Method
dvisc	0.0000284	Paxs	678.40	Joback Method
dvisc	0.0000195	Paxs	718.06	Joback Method
dvisc	0.0000139	Paxs	757.71	Joback Method
dvisc	0.0000102	Paxs	797.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92153178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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