

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

Inchi:	InChI=1S/C16H14Cl2O2/c1-9(2)10-4-6-15(19)12(7-10)16(20)11-3-5-13(17)14(18)8-11/h3
InchiKey:	XXAJPJDOUPKTPR-UHFFFAOYSA-N
Formula:	C16H14Cl2O2
SMILES:	CC(C)c1ccc(O)c(C(=O)c2ccc(Cl)c(Cl)c2)c1
Mol. weight [g/mol]:	309.19
CAS:	116495-89-7

Physical Properties

Property code	Value	Unit	Source
gf	-30.07	kJ/mol	Joback Method
hf	-261.57	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	85.89	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.053		Crippen Method
mcvol	220.700	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
tb	842.69	K	Joback Method
tc	1096.61	K	Joback Method
tf	566.97	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.88	J/molxK	842.69	Joback Method
cpg	640.23	J/molxK	1054.29	Joback Method
cpg	630.06	J/molxK	1011.97	Joback Method
cpg	619.57	J/molxK	969.65	Joback Method
cpg	608.64	J/molxK	927.33	Joback Method
cpg	597.12	J/molxK	885.01	Joback Method
cpg	650.22	J/molxK	1096.61	Joback Method
dvisc	0.0000063	Paxs	842.69	Joback Method
dvisc	0.0000088	Paxs	796.74	Joback Method

dvisc	0.0000128	Paxs	750.78	Joback Method
dvisc	0.0000196	Paxs	704.83	Joback Method
dvisc	0.0000317	Paxs	658.88	Joback Method
dvisc	0.0000551	Paxs	612.92	Joback Method
dvisc	0.0001049	Paxs	566.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495897&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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