

3',4'-Dichloro-4,5-dimethyl-2-hydroxy benzophenone

Inchi:	InChI=1S/C15H12Cl2O2/c1-8-5-11(14(18)6-9(8)2)15(19)10-3-4-12(16)13(17)7-10/h3-7,1
InchiKey:	GRGXTVBGKMCVJJ-UHFFFAOYSA-N
Formula:	C15H12Cl2O2
SMILES:	Cc1cc(O)c(C(=O)c2ccc(Cl)c(Cl)c2)cc1C
Mol. weight [g/mol]:	295.16

Physical Properties

Property code	Value	Unit	Source
gf	-45.68	kJ/mol	Joback Method
hf	-247.12	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.547		Crippen Method
mcvol	206.610	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	825.23	K	Joback Method
tc	1080.41	K	Joback Method
tf	583.22	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.60	J/molxK	825.23	Joback Method
cpg	580.41	J/molxK	1037.88	Joback Method
cpg	570.91	J/molxK	995.35	Joback Method
cpg	561.10	J/molxK	952.82	Joback Method
cpg	550.86	J/molxK	910.29	Joback Method
cpg	540.06	J/molxK	867.76	Joback Method
cpg	589.71	J/molxK	1080.41	Joback Method
dvisc	0.0000084	Paxs	825.23	Joback Method
dvisc	0.0000112	Paxs	784.89	Joback Method
dvisc	0.0000155	Paxs	744.56	Joback Method

dvisc	0.0000222	Paxs	704.23	Joback Method
dvisc	0.0000332	Paxs	663.89	Joback Method
dvisc	0.0000525	Paxs	623.56	Joback Method
dvisc	0.0000883	Paxs	583.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004193&Units=SI
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

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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