

Benzophenone, 5-chloro-4-dodecyloxy-2-hydroxy-4'-methoxy-

Inchi:	InChI=1S/C26H35ClO4/c1-3-4-5-6-7-8-9-10-11-12-17-31-25-19-24(28)22(18-23(25)27)2
InchiKey:	ZBNHYEUPIXLEK-UHFFFAOYSA-N
Formula:	C26H35ClO4
SMILES:	CCCCCCCCCCCCOc1cc(O)c(C(=O)c2ccc(OC)cc2)cc1Cl
Mol. weight [g/mol]:	447.01
CAS:	116400-88-5

Physical Properties

Property code	Value	Unit	Source
gf	-141.50	kJ/mol	Joback Method
hf	-711.39	kJ/mol	Joback Method
hfus	63.97	kJ/mol	Joback Method
hvap	108.97	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.585		Crippen Method
mcvol	361.100	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
tb	1079.34	K	Joback Method
tc	1321.46	K	Joback Method
tf	709.21	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.60	J/molxK	1079.34	Joback Method
cpg	1221.46	J/molxK	1119.69	Joback Method
cpg	1236.39	J/molxK	1160.05	Joback Method
cpg	1250.50	J/molxK	1200.40	Joback Method
cpg	1263.91	J/molxK	1240.75	Joback Method
cpg	1276.73	J/molxK	1281.11	Joback Method
cpg	1289.10	J/molxK	1321.46	Joback Method
dvisc	0.0000104	Paxs	709.21	Joback Method
dvisc	0.0000054	Paxs	770.90	Joback Method

dvisc	0.0000031	Paxs	832.59	Joback Method
dvisc	0.0000019	Paxs	894.27	Joback Method
dvisc	0.0000012	Paxs	955.96	Joback Method
dvisc	0.0000009	Paxs	1017.65	Joback Method
dvisc	0.0000006	Paxs	1079.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116400885&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

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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