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)26

InchiKey: ZBNHYEUPICXLEK-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/mol×K	1079.34	Joback Method
cpg	1276.73	J/mol×K	1281.11	Joback Method
cpg	1263.91	J/mol×K	1240.75	Joback Method
cpg	1250.50	J/mol×K	1200.40	Joback Method
cpg	1236.39	J/mol×K	1160.05	Joback Method
cpg	1221.46	J/mol×K	1119.69	Joback Method
cpg	1289.10	J/mol×K	1321.46	Joback Method
dvisc	0.0000006	Pa×s	1079.34	Joback Method
dvisc	0.0000009	Pa×s	1017.65	Joback Method

dvisc	0.0000012	Pa×s	955.96	Joback Method
dvisc	0.0000019	Pa×s	894.27	Joback Method
dvisc	0.0000031	Pa×s	832.59	Joback Method
dvisc	0.0000054	Pa×s	770.90	Joback Method
dvisc	0.0000104	Pa×s	709.21	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116400885&Units=SI

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