Benzophenone, 2,4-dihydroxy-4'-methyl

Other names: 2,4-dihydroxy-4'-methylbenzophenone
Inchi: InChI=1S/C14H12O3/c1-9-2-4-10(5-3-9)14(17)12-7-6-11(15)8-13(12)16/h2-8,15-16H,1H
InchiKey: FGCATPMSNCVLQK-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: Cc1ccc(C(=O)c2ccc(O)cc2O)cc1
Mol. weight [g/mol]: 228.24
CAS: 40444-43-7

Physical Properties

Property code	Value	Unit	Source
gf	-155.97	kJ/mol	Joback Method
hf	-337.90	kJ/mol	Joback Method
hfus	32.87	kJ/mol	Joback Method
hvap	84.75	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.637		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	793.17	K	Joback Method
tc	1053.98	K	Joback Method
tf	586.27	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.65	J/mol×K	793.17	Joback Method
cpg	538.11	J/mol×K	1010.52	Joback Method
cpg	526.90	J/mol×K	967.05	Joback Method
cpg	515.87	J/mol×K	923.58	Joback Method
cpg	504.80	J/mol×K	880.11	Joback Method
cpg	493.46	J/mol×K	836.64	Joback Method
cpg	549.70	J/mol×K	1053.98	Joback Method
dvisc	0.0000008	Pa×s	793.17	Joback Method

dvisc	0.0000011	Pa×s	758.69	Joback Method
dvisc	0.0000017	Pa×s	724.20	Joback Method
dvisc	0.0000028	Pa×s	689.72	Joback Method
dvisc	0.0000047	Pa×s	655.24	Joback Method
dvisc	0.0000085	Pa×s	620.75	Joback Method
dvisc	0.0000163	Pa×s	586.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40444437&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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