Benzophenone, 2,4-dihydroxy-4-benzoate

Inchi: InChI=1S/C20H14O4/c21-18-13-16(24-20(23)15-9-5-2-6-10-15)11-12-17(18)19(22)14-7-
InchiKey: CNAILFQALPMJFF-UHFFFAOYSA-N
Formula: C20H14O4
SMILES: O=C(Oc1ccc(C(=O)c2ccccc2)c(O)c1)c1ccccc1
Mol. weight [g/mol]: 318.32
CAS: 18803-25-3

Physical Properties

Property code	Value	Unit	Source
gf	-72.34	kJ/mol	Joback Method
hf	-292.70	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	96.52	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.842		Crippen Method
mcvol	236.260	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	952.80	K	Joback Method
tc	1219.02	K	Joback Method
tf	640.75	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.71	J/mol×K	952.80	Joback Method
cpg	710.75	J/mol×K	997.17	Joback Method
cpg	722.06	J/mol×K	1041.54	Joback Method
cpg	732.81	J/mol×K	1085.91	Joback Method
cpg	743.19	J/mol×K	1130.28	Joback Method
cpg	753.37	J/mol×K	1174.65	Joback Method
cpg	763.53	J/mol×K	1219.02	Joback Method
dvisc	0.0000443	Pa×s	640.75	Joback Method
dvisc	0.0000236	Pa×s	692.76	Joback Method

dvisc	0.0000137	Pa×s	744.77	Joback Method
dvisc	0.0000086	Pa×s	796.77	Joback Method
dvisc	0.0000057	Pa×s	848.78	Joback Method
dvisc	0.0000039	Pa×s	900.79	Joback Method
dvisc	0.0000028	Pa×s	952.80	Joback Method

Sources

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=C18803253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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