

3',4'-Dihydroxybutyrophenone

Inchi:	InChI=1S/C10H12O3/c1-2-3-8(11)7-4-5-9(12)10(13)6-7/h4-6,12-13H,2-3H2,1H3
InchiKey:	NLERVTXJOGYIKC-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCCC(=O)c1ccc(O)c(O)c1
Mol. weight [g/mol]:	180.20
CAS:	17386-89-9

Physical Properties

Property code	Value	Unit	Source
gf	-292.43	kJ/mol	Joback Method
hf	-480.40	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.081		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	669.99	K	Joback Method
tc	905.37	K	Joback Method
tf	502.25	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.16	J/molxK	669.99	Joback Method
cpg	382.81	J/molxK	709.22	Joback Method
cpg	392.80	J/molxK	748.45	Joback Method
cpg	402.26	J/molxK	787.68	Joback Method
cpg	411.36	J/molxK	826.91	Joback Method
cpg	420.21	J/molxK	866.14	Joback Method
cpg	428.97	J/molxK	905.37	Joback Method
dvisc	0.0000813	Paxs	502.25	Joback Method
dvisc	0.0000408	Paxs	530.21	Joback Method

dvisc	0.0000220	Paxs	558.16	Joback Method
dvisc	0.0000126	Paxs	586.12	Joback Method
dvisc	0.0000075	Paxs	614.08	Joback Method
dvisc	0.0000047	Paxs	642.03	Joback Method
dvisc	0.0000031	Paxs	669.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C17386899&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

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