

3,4-Dihydroxyacetophenone

Other names:	3',4'-Dihydroxyacetophenone Ethanone, 1-(3,4-dihydroxyphenyl)-
Inchi:	InChI=1S/C8H8O3/c1-5(9)6-2-3-7(10)8(11)4-6/h2-4,10-11H,1H3
InchiKey:	UCQUAMAQHHXGD-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	CC(=O)c1ccc(O)c(O)c1
Mol. weight [g/mol]:	152.15
CAS:	1197-09-7

Physical Properties

Property code	Value	Unit	Source
gf	-309.27	kJ/mol	Joback Method
hf	-439.12	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.300		Crippen Method
mvol	113.130	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
tb	624.23	K	Joback Method
tc	869.83	K	Joback Method
tf	479.71	K	Joback Method
vc	0.314	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.53	J/molxK	624.23	Joback Method
cpg	317.34	J/molxK	828.90	Joback Method
cpg	310.35	J/molxK	787.96	Joback Method
cpg	303.12	J/molxK	747.03	Joback Method
cpg	295.51	J/molxK	706.10	Joback Method
cpg	287.36	J/molxK	665.16	Joback Method
cpg	324.25	J/molxK	869.83	Joback Method

dvisc	0.0000059	Paxs	624.23	Joback Method
dvisc	0.0000089	Paxs	600.14	Joback Method
dvisc	0.0000138	Paxs	576.06	Joback Method
dvisc	0.0000224	Paxs	551.97	Joback Method
dvisc	0.0000380	Paxs	527.88	Joback Method
dvisc	0.0000676	Paxs	503.80	Joback Method
dvisc	0.0001275	Paxs	479.71	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=C1197097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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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