

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:	UCQUAMAQHHEXGD-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/mol×K	624.23	Joback Method
cpg	287.36	J/mol×K	665.16	Joback Method
cpg	295.51	J/mol×K	706.10	Joback Method
cpg	303.12	J/mol×K	747.03	Joback Method
cpg	310.35	J/mol×K	787.96	Joback Method
cpg	317.34	J/mol×K	828.90	Joback Method
cpg	324.25	J/mol×K	869.83	Joback Method

dvisc	0.0001275	Paxs	479.71	Joback Method
dvisc	0.0000676	Paxs	503.80	Joback Method
dvisc	0.0000380	Paxs	527.88	Joback Method
dvisc	0.0000224	Paxs	551.97	Joback Method
dvisc	0.0000138	Paxs	576.06	Joback Method
dvisc	0.0000089	Paxs	600.14	Joback Method
dvisc	0.0000059	Paxs	624.23	Joback Method

Sources

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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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