2,3-dihydroxyacetophenone

Inchi: InChI=1S/C8H8O3/c1-5(9)6-3-2-4-7(10)8(6)11/h2-4,10-11H,1H3
InchiKey: HEJLFBLJYFSKCE-UHFFFAOYSA-N
Formula: C8H8O3
SMILES: CC(=O)c1cccc(O)c1O
Mol. weight [g/mol]: 152.15

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
mcvol	113.130	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
rinpol	1255.00		NIST Webbook
rinpol	1255.00		NIST Webbook
tb	624.23	K	Joback Method
tc	869.83	K	Joback Method
tf	479.71	K	Joback Method
vc	0.314	m3/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	Pa×s	479.71	Joback Method

dvisc	0.0000676	Pa×s	503.80	Joback Method
dvisc	0.0000380	Pa×s	527.88	Joback Method
dvisc	0.0000224	Pa×s	551.97	Joback Method
dvisc	0.0000138	Pa×s	576.06	Joback Method
dvisc	0.0000089	Pa×s	600.14	Joback Method
dvisc	0.0000059	Pa×s	624.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R230381&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume