2',6'-DIHYDROXYACETOPHENONE

Other names:	2',6'-Dihydroxyacetophenone 2,6-Dihydroxyacetophenone 2-Acetylresorcinol Acetyl-2,6-dihydroxybenzene Ethanone, 1-(2,6-dihydroxyphenyl)- «gamma»-Resacetophenone Acetophenone, 2',6'-dihydroxy- 1,3-Benzenediol, 2-acetyl- 1-(2,6-Dihydroxyphenyl)ethanone NSC 615
Inchi:	InChI=1S/C8H8O3/c1-5(9)8-6(10)3-2-4-7(8)11/h2-4,10-11H,1H3
InchiKey:	YPTJKHVBDCRKNF-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	CC(=O)c1c(O)cccc1O
Mol. weight [g/mol]:	152.15

Physical Properties

Property code	Value	Unit	Source
af	0.6880		Cheméo Relay (1.0)
gf	-309.27	kJ/mol	Joback Method
hf	-458.55	kJ/mol	Cheméo Relay (1.0)
hfus	23.68	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.300		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
tb	537.75	K	Cheméo Relay (1.0)
tc	812.31	K	Cheméo Relay (1.0)
tf	339.78	K	Cheméo Relay (1.0)
vc	0.388	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C699832&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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
ie:	Ionization energy
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