2',4'-DIHYDROXYACETOPHENONE

Other names:	1-(2,4-Dihydroxyphenyl)ethanone 1-Acetylbenzene-2,4-diol 2',4'-Dihydroxyacetophenone 2,4-Dihydroxyacetophenone 4-Acetyl-1,3-benzenediol 4-Acetylresorcinol Acetophenone, 2',4'-dihydroxy- NSC 10883 Resacetophenone Resoacetophenone Resorcinol, 4-acetyl- beta-Resacetophenone «beta»-Resacetophenone
Inchi:	InChI=1S/C8H8O3/c1-5(9)7-3-2-6(10)4-8(7)11/h2-4,10-11H,1H3
InchiKey:	SULYEHHGGXARJS-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	CC(=O)c1ccc(O)cc1O
Mol. weight [g/mol]:	152.15

Physical Properties

Property code	Value	Unit	Source
chs	-3717.90 ± 3.80	kJ/mol	NIST Webbook
hf	-469.04	kJ/mol	Cheméo Relay (1.0)
hfus	23.68	kJ/mol	Joback Method
hvap	91.43	kJ/mol	Cheméo Relay (1.0)
ie	8.49	eV	Cheméo Relay (1.0)
log10ws	-1.56		Cheméo Relay (1.0)
logp	1.300		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
tb	563.04	K	Cheméo Relay (1.0)
tf	396.35	K	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=C89849&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

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point