3,4-DIHYDROXY-5-METHOXYBENZALDEHYDE

Other names:	5-Hydroxyvanillin
	5-Methoxyprotocatechualdehyde
	Benzaldehyde, 3,4-dihydroxy-5-methoxy-
	Protocatechualdehyde, 5-methoxy-
Inchi:	InChI=1S/C8H8O4/c1-12-7-3-5(4-9)2-6(10)8(7)11/h2-4,10-11H,1H3
InchiKey:	RRKMWVISRMWBAL-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	COc1cc(C=O)cc(O)c1O
Mol. weight [g/mol]:	168.15

Physical Properties

Property code	Value	Unit	Source
hfus	25.17	kJ/mol	Joback Method
hvap	104.24	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.04		Cheméo Relay (1.0)
logp	0.919		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
tb	569.85	K	Cheméo Relay (1.0)
tf	404.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.41	J/mol×K	646.42	Joback Method
cpg	307.75	J/mol×K	685.97	Joback Method
cpg	315.58	J/mol×K	725.52	Joback Method
cpg	323.00	J/mol×K	765.07	Joback Method
cpg	330.12	J/mol×K	804.61	Joback Method
cpg	337.05	J/mol×K	844.16	Joback Method
cpg	343.90	J/mol×K	883.71	Joback Method
dvisc	0.0000631	Pa×s	506.53	Joback Method
dvisc	0.0000362	Pa×s	529.85	Joback Method
dvisc	0.0000218	Pa×s	553.16	Joback Method
dvisc	0.0000137	Pa×s	576.48	Joback Method

dvisc	0.0000089	Pa×s	599.79	Joback Method
dvisc	0.0000060	Pa×s	623.11	Joback Method
dvisc	0.0000041	Pa×s	646.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3934870&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point