3,4-Dihydroxy-5-methoxybenzaldehyde

Other names:	Benzaldehyde, 3,4-dihydroxy-5-methoxy- Protocatechualdehyde, 5-methoxy- 5-Methoxyprotocatechualdehyde 5-Hydroxyvanillin
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
CAS:	3934-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-394.50	kJ/mol	Joback Method
hf	-555.81	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	0.919		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	5782.94	kPa	Joback Method
tb	646.42	K	Joback Method
tc	883.71	K	Joback Method
tf	506.53	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.41	J/mol×K	646.42	Joback Method
cpg	337.05	J/mol×K	844.16	Joback Method
cpg	330.12	J/mol×K	804.61	Joback Method
cpg	323.00	J/mol×K	765.07	Joback Method
cpg	315.58	J/mol×K	725.52	Joback Method

cpg	307.75	J/mol×K	685.97	Joback Method
cpg	343.90	J/mol×K	883.71	Joback Method
dvisc	0.0000041	Pa×s	646.42	Joback Method
dvisc	0.0000060	Pa×s	623.11	Joback Method
dvisc	0.0000089	Pa×s	599.79	Joback Method
dvisc	0.0000137	Pa×s	576.48	Joback Method
dvisc	0.0000218	Pa×s	553.16	Joback Method
dvisc	0.0000362	Pa×s	529.85	Joback Method
dvisc	0.0000631	Pa×s	506.53	Joback Method

Sources

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=C3934870&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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