3-Hydroxy-4,5-dimethoxybenzoic acid

Other names:	3,4-Dimethoxy-5-hydroxy benzoic acid
	5-Hydroxy veratric acid
	5-Hydroxy-3,4-dimethoxybenzoic acid
	Benzoic acid, 3-hydroxy-4,5-dimethoxy-
Inchi:	InChI=1S/C9H10O5/c1-13-7-4-5(9(11)12)3-6(10)8(7)14-2/h3-4,10H,1-2H3,(H,11,12)
InchiKey:	WFIBQVFJXGQICQ-UHFFFAOYSA-N
Formula:	C9H10O5
SMILES:	COc1cc(C(=O)O)cc(O)c1OC
Mol. weight [g/mol]:	198.17
CAS:	1916-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-512.31	kJ/mol	Joback Method
hf	-722.06	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	80.49	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.108		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	713.47	K	Joback Method
tc	923.84	K	Joback Method
tf	509.58	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.72	J/mol×K	713.47	Joback Method
cpg	406.19	J/mol×K	888.78	Joback Method
cpg	399.15	J/mol×K	853.72	Joback Method
cpg	391.71	J/mol×K	818.66	Joback Method
cpg	383.84	J/mol×K	783.59	Joback Method

cpg	375.52	J/mol×K	748.53	Joback Method
cpg	412.86	J/mol×K	923.84	Joback Method
dvisc	0.0000039	Pa×s	713.47	Joback Method
dvisc	0.0000059	Pa×s	679.49	Joback Method
dvisc	0.0000092	Pa×s	645.51	Joback Method
dvisc	0.0000152	Pa×s	611.53	Joback Method
dvisc	0.0000265	Pa×s	577.54	Joback Method
dvisc	0.0000498	Pa×s	543.56	Joback Method
dvisc	0.0001015	Pa×s	509.58	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1916081&Units=SI
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

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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