3,5-Dihydroxy-4-methoxybenzoic acid

Other names:	4-O-Methylgallic acid
	3,5-Dihydroxy-4-methoxybenzoic acid
	5-Hydroxyisovanillic acid
	Benzoic acid, 3,5-dihydroxy-4-methoxy-
	3,5-dihydroxy-p-anisic acid
Inchi:	InChI=1S/C8H8O5/c1-13-7-5(9)2-4(8(11)12)3-6(7)10/h2-3,9-10H,1H3,(H,11,12)
InchiKey:	UBXDWYFLYYJQFR-UHFFFAOYSA-N
Formula:	C8H8O5
SMILES:	COc1c(O)cc(C(=O)O)cc1O
Mol. weight [g/mol]:	184.15

Physical Properties

Property code	Value	Unit	Source
hf	-774.74	kJ/mol	Cheméo Relay (1.0)
hfus	28.57	kJ/mol	Joback Method
hvap	122.62	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	0.805		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
tb	567.74	K	Cheméo Relay (1.0)
tf	496.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.57	J/mol×K	743.81	Joback Method
cpg	341.70	J/mol×K	780.98	Joback Method
cpg	348.58	J/mol×K	818.15	Joback Method
cpg	355.29	J/mol×K	855.32	Joback Method
cpg	361.92	J/mol×K	892.49	Joback Method
cpg	368.57	J/mol×K	929.66	Joback Method
cpg	375.33	J/mol×K	966.83	Joback Method
dvisc	0.0000083	Pa×s	575.28	Joback Method

dvisc	0.0000043	Pa×s	603.37	Joback Method
dvisc	0.0000024	Pa×s	631.46	Joback Method
dvisc	0.0000014	Pa×s	659.54	Joback Method
dvisc	0.0000008	Pa×s	687.63	Joback Method
dvisc	0.0000005	Pa×s	715.72	Joback Method
dvisc	0.0000003	Pa×s	743.81	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4319022&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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