3-Hydroxy-4-methoxybenzoic acid

Other names:	Isovanillic acid
	Benzoic acid, 3-hydroxy-4-methoxy-
	p-Anisic acid, 3-hydroxy-
	Acide isovanillique
	3-Hydroxyanisic acid
	3-hydroxy-p-anisic acid
Inchi:	InChI=1S/C8H8O4/c1-12-7-3-2-5(8(10)11)4-6(7)9/h2-4,9H,1H3,(H,10,11)
InchiKey:	LBKFGYZQBSGRHY-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	COc1ccc(C(=O)O)cc1O
Mol. weight [g/mol]:	168.15
CAS:	645-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-406.10	kJ/mol	Joback Method
hf	-557.73	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	75.19	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.099		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	5228.24	kPa	Joback Method
tb	663.19	K	Joback Method
tc	878.05	K	Joback Method
tf	523.15 ± 3.00	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.09	J/mol×K	663.19	Joback Method
cpg	333.98	J/mol×K	842.24	Joback Method
cpg	327.60	J/mol×K	806.43	Joback Method

cpg	320.86	J/mol×K	770.62	Joback Method
cpg	313.72	J/mol×K	734.81	Joback Method
cpg	306.15	J/mol×K	699.00	Joback Method
cpg	340.07	J/mol×K	878.05	Joback Method
dvisc	0.0000078	Pa×s	663.19	Joback Method
dvisc	0.0000123	Pa×s	629.92	Joback Method
dvisc	0.0000202	Pa×s	596.65	Joback Method
dvisc	0.0000353	Pa×s	563.38	Joback Method
dvisc	0.0000663	Pa×s	530.10	Joback Method
dvisc	0.0001353	Pa×s	496.83	Joback Method
dvisc	0.0003059	Pa×s	463.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645089&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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