Benzeneacetic acid, 4-hydroxy-3-methoxy-, methyl ester

Other names:	Acetic acid, (4-hydroxy-3-methoxyphenyl)-, methyl ester
	Homovanillic acid methyl ester
	Methyl 3-methoxy-4-hydroxyphenylacetate
	Methyl homovanillate
	methyl 4-hydroxy-3-methoxyphenylacetate
Inchi:	InChI=1S/C10H12O4/c1-13-9-5-7(3-4-8(9)11)6-10(12)14-2/h3-5,11H,6H2,1-2H3
InchiKey:	JJJSFAGPWHEUBT-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COC(=O)Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	196.20
CAS:	15964-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-357.44	kJ/mol	Joback Method
hf	-579.00	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.116		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	639.19	K	Joback Method
tc	860.68	K	Joback Method
tf	447.51	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.77	J/mol×K	639.19	Joback Method
cpg	384.49	J/mol×K	676.10	Joback Method
cpg	395.53	J/mol×K	713.02	Joback Method
cpg	405.91	J/mol×K	749.93	Joback Method

cpg	415.69	J/mol×K	786.85	Joback Method
cpg	424.90	J/mol×K	823.76	Joback Method
cpg	433.57	J/mol×K	860.68	Joback Method
dvisc	0.0003718	Pa×s	447.51	Joback Method
dvisc	0.0001978	Pa×s	479.46	Joback Method
dvisc	0.0001139	Pa×s	511.40	Joback Method
dvisc	0.0000700	Pa×s	543.35	Joback Method
dvisc	0.0000454	Pa×s	575.30	Joback Method
dvisc	0.0000308	Pa×s	607.24	Joback Method
dvisc	0.0000217	Pa×s	639.19	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=C15964804&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