Benzeneacetic acid, 3-hydroxy-, methyl ester

Other names:	Methyl m-hydroxyphenylacetate
	Methyl (3-hydroxyphenyl)acetate
Inchi:	InChI=1S/C9H10O3/c1-12-9(11)6-7-3-2-4-8(10)5-7/h2-5,10H,6H2,1H3
InchiKey:	AMDDOQIUPAINLH-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(=O)Cc1cccc(O)c1
Mol. weight [g/mol]:	166.17
CAS:	42058-59-3

Physical Properties

Property code	Value	Unit	Source
gf	-251.23	kJ/mol	Joback Method
hf	-414.67	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.108		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1449.00		NIST Webbook
tb	588.91	K	Joback Method
tc	816.64	K	Joback Method
tf	401.49	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.03	J/mol×K	588.91	Joback Method
cpg	353.29	J/mol×K	778.68	Joback Method
cpg	344.71	J/mol×K	740.73	Joback Method
cpg	335.56	J/mol×K	702.77	Joback Method
cpg	325.77	J/mol×K	664.82	Joback Method
cpg	315.28	J/mol×K	626.86	Joback Method

cpg	361.35	J/mol×K	816.64	Joback Method
dvisc	0.0000400	Pa×s	588.91	Joback Method
dvisc	0.0000590	Pa×s	557.67	Joback Method
dvisc	0.0000909	Pa×s	526.44	Joback Method
dvisc	0.0001481	Pa×s	495.20	Joback Method
dvisc	0.0002577	Pa×s	463.96	Joback Method
dvisc	0.0004856	Pa×s	432.73	Joback Method
dvisc	0.0010100	Pa×s	401.49	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=C42058593&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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