Benzenepropanoic acid, «alpha»-hydroxy-4-methoxy-, methyl ester

Other names: Propanoic acid, 2-hydroxy-3-(4-methoxyphenyl), methyl ester
Lactic acid, 3-(p-methoxyphenyl)-, methyl ester

Inchi: InChI=1S/C11H14O4/c1-14-9-5-3-8(4-6-9)7-10(12)11(13)15-2/h3-6,10,12H,7H2,1-2H3

InchiKey: LDDFEROTLHOWEW-UHFFFAOYSA-N

Formula: C11H14O4

SMILES: COC(=O)C(O)Cc1ccc(OC)cc1

Mol. weight [g/mol]: 210.23

CAS: 55301-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-333.66	kJ/mol	Joback Method
hf	-579.84	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	70.88	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	0.772		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	673.19	K	Joback Method
tc	872.12	K	Joback Method
tf	392.88	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.11	J/mol×K	673.19	Joback Method

cpg	435.85	J/mol×K	706.34	Joback Method
cpg	446.91	J/mol×K	739.50	Joback Method
cpg	457.29	J/mol×K	772.65	Joback Method
cpg	467.00	J/mol×K	805.81	Joback Method
cpg	476.04	J/mol×K	838.96	Joback Method
cpg	484.42	J/mol×K	872.12	Joback Method
dvisc	0.0017217	Pa×s	392.88	Joback Method
dvisc	0.0006544	Pa×s	439.60	Joback Method
dvisc	0.0002995	Pa×s	486.32	Joback Method
dvisc	0.0001572	Pa×s	533.04	Joback Method
dvisc	0.0000916	Pa×s	579.75	Joback Method
dvisc	0.0000578	Pa×s	626.47	Joback Method
dvisc	0.0000389	Pa×s	673.19	Joback Method

Sources

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=C55301581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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