Benzenebutanoic acid, 4-hydroxy-, methyl ester

Other names: Butyric acid, 4-(p-hydroxyphenyl)-, methyl ester
4-(p-Hydroxyphenyl)butyric acid methyl ester
Methyl 4-(4-hydroxyphenyl)butanoate
4-(4-Hydroxyphenyl)butanoic acid methyl ester

Inchi: InChI=1S/C11H14O3/c1-14-11(13)4-2-3-9-5-7-10(12)8-6-9/h5-8,12H,2-4H2,1H3

InchiKey: UZHISWLCHOMTIO-UHFFFAOYSA-N

Formula: C11H14O3

SMILES: COC(=O)CCCc1ccc(O)cc1

Mol. weight [g/mol]: 194.23

CAS: 22320-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-234.39	kJ/mol	Joback Method
hf	-455.95	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
ie	8.50 ± 0.20	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.888		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	634.67	K	Joback Method
tc	854.09	K	Joback Method
tf	424.03	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.53	J/mol×K	634.67	Joback Method
cpg	455.33	J/mol×K	817.52	Joback Method
cpg	445.32	J/mol×K	780.95	Joback Method
cpg	434.71	J/mol×K	744.38	Joback Method

cpg	423.41	J/mol×K	707.81	Joback Method
cpg	411.37	J/mol×K	671.24	Joback Method
cpg	464.78	J/mol×K	854.09	Joback Method
dvisc	0.0000257	Pa×s	634.67	Joback Method
dvisc	0.0000380	Pa×s	599.56	Joback Method
dvisc	0.0000592	Pa×s	564.46	Joback Method
dvisc	0.0000977	Pa×s	529.35	Joback Method
dvisc	0.0001730	Pa×s	494.24	Joback Method
dvisc	0.0003344	Pa×s	459.14	Joback Method
dvisc	0.0007210	Pa×s	424.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22320101&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
ie: Ionization energy
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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