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

Other names: Mandelic acid, p-methoxy-, methyl ester
Methyl p-methoxymandelate
Acetic acid, «alpha»-hydroxy-«alpha»-(4-methoxyphenyl), methyl ester
Acetic acid, hydroxy-(4-methoxyphenyl), methyl ester
Methyl 4-methoxymandelate

Inchi: InChI=1S/C10H12O4/c1-13-8-5-3-7(4-6-8)9(11)10(12)14-2/h3-6,9,11H,1-2H3

InchiKey: RXVKSXZEZOODTF-UHFFFAOYSA-N

Formula: C10H12O4

SMILES: COC(=O)C(O)c1ccc(OC)cc1

Mol. weight [g/mol]: 196.20

CAS: 13305-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-342.08	kJ/mol	Joback Method
hf	-559.20	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.902		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	650.31	K	Joback Method
tc	851.71	K	Joback Method
tf	381.61	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.48	J/mol×K	650.31	Joback Method

cpg	385.54	J/mol×K	683.88	Joback Method
cpg	395.98	J/mol×K	717.44	Joback Method
cpg	405.80	J/mol×K	751.01	Joback Method
cpg	414.98	J/mol×K	784.57	Joback Method
cpg	423.53	J/mol×K	818.14	Joback Method
cpg	431.45	J/mol×K	851.71	Joback Method
dvisc	0.0020044	Pa×s	381.61	Joback Method
dvisc	0.0007688	Pa×s	426.39	Joback Method
dvisc	0.0003538	Pa×s	471.18	Joback Method
dvisc	0.0001863	Pa×s	515.96	Joback Method
dvisc	0.0001087	Pa×s	560.74	Joback Method
dvisc	0.0000686	Pa×s	605.53	Joback Method
dvisc	0.0000462	Pa×s	650.31	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13305141&Units=SI

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