Benzeneacetic acid, «alpha»-cyclopentyl-«alpha»-hydroxy-, methyl ester

Othernames: Cyclopentyl(hydroxy)phenylacetic acid, methyl ester
Methyl cyclopentyl(hydroxy)phenylacetate
«alpha»-Cyclopentylmandelic acid, methyl ester
Mandelic acid, a-cyclopentyl-, methyl ester
Methyl cyclopentylphenylglycolate
Alpha-cyclopentylmandelic acid, methyl ester

Inchi: InChI=1S/C14H18O3/c1-17-13(15)14(16,12-9-5-6-10-12)11-7-3-2-4-8-11/h2-4,7-8,12,16H

InchiKey: FGMUSNHTKNGVQD-UHFFFAOYSA-N

Formula: C14H18O3

SMILES: COC(=O)C(O)(c1ccccc1)C1CCCC1

Mol. weight [g/mol]: 234.29

CAS: 19833-96-6

Physical Properties

Property code	Value	Unit	Source
gf	-151.94	kJ/mol	Joback Method
hf	-441.06	kJ/mol	Joback Method
hfus	19.45	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.237		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
tb	726.92	K	Joback Method
tc	948.92	K	Joback Method
tf	420.26	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.82	J/mol×K	726.92	Joback Method
cpg	561.91	J/mol×K	763.92	Joback Method
cpg	575.85	J/mol×K	800.92	Joback Method

cpg	588.71	J/mol×K	837.92	Joback Method
cpg	600.55	J/mol×K	874.92	Joback Method
cpg	611.44	J/mol×K	911.92	Joback Method
cpg	621.48	J/mol×K	948.92	Joback Method
dvisc	0.0020171	Pa×s	420.26	Joback Method
dvisc	0.0007372	Pa×s	471.37	Joback Method
dvisc	0.0003281	Pa×s	522.48	Joback Method
dvisc	0.0001687	Pa×s	573.59	Joback Method
dvisc	0.0000967	Pa×s	624.70	Joback Method
dvisc	0.0000603	Pa×s	675.81	Joback Method
dvisc	0.0000402	Pa×s	726.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19833966&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

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

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