Cyclopentyl(hydroxy)phenylacetic acid, methyl ester

Other names: Alpha-cyclopentylmandelic acid, methyl ester
Cyclopentyl(hydroxy)phenylacetic acid, methyl ester
Mandelic acid, a-cyclopentyl-, methyl ester
Methyl cyclopentyl(hydroxy)phenylacetate
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]: 234.30

Physical Properties

Property code	Value	Unit	Source
hfus	19.45	kJ/mol	Joback Method
logp	2.237		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
tb	575.40	K	Cheméo Relay (1.0)
tf	331.50	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19833966&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point