2-[4-(1-Hydroxy-2-methylpropyl)phenyl]propanoic acid, monomethyl

Inchi: InChI=1S/C14H20O3/c1-9(2)13(15)12-7-5-11(6-8-12)10(3)14(16)17-4/h5-10,13,15H,1-4H

InchiKey: JBMWZTVMWRQDEK-UHFFFAOYSA-N

Formula: C14H20O3

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

Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-208.28	kJ/mol	Joback Method
hf	-520.10	kJ/mol	Joback Method
hfus	21.97	kJ/mol	Joback Method
hvap	74.37	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.652		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1709.00		NIST Webbook
tb	718.53	K	Joback Method
tc	918.85	K	Joback Method
tf	374.46	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.43	J/mol×K	718.53	Joback Method
cpg	569.41	J/mol×K	751.92	Joback Method
cpg	582.53	J/mol×K	785.30	Joback Method
cpg	594.81	J/mol×K	818.69	Joback Method
cpg	606.27	J/mol×K	852.08	Joback Method
cpg	616.94	J/mol×K	885.46	Joback Method
cpg	626.84	J/mol×K	918.85	Joback Method
dvisc	0.0035231	Pa×s	374.46	Joback Method
dvisc	0.0009115	Pa×s	431.81	Joback Method

dvisc	0.0003238	Pa×s	489.15	Joback Method
dvisc	0.0001429	Pa×s	546.50	Joback Method
dvisc	0.0000737	Pa×s	603.84	Joback Method
dvisc	0.0000426	Pa×s	661.19	Joback Method
dvisc	0.0000269	Pa×s	718.53	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=R399490&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