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

Inchi: InChI=1S/C15H22O3/c1-10(2)14(17-4)13-8-6-12(7-9-13)11(3)15(16)18-5/h6-11,14H,1-5H

InchiKey: WNKBIUUWCXJTCQ-UHFFFAOYSA-N

Formula: C15H22O3

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

Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-168.04	kJ/mol	Joback Method
hf	-520.73	kJ/mol	Joback Method
hfus	21.66	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.307		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	671.65	K	Joback Method
tc	879.13	K	Joback Method
tf	347.14	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.43	J/mol×K	671.65	Joback Method
cpg	651.52	J/mol×K	844.55	Joback Method
cpg	638.28	J/mol×K	809.97	Joback Method
cpg	624.07	J/mol×K	775.39	Joback Method
cpg	608.86	J/mol×K	740.81	Joback Method
cpg	592.65	J/mol×K	706.23	Joback Method
cpg	663.79	J/mol×K	879.13	Joback Method
dvisc	0.0000843	Pa×s	671.65	Joback Method

dvisc	0.0001139	Pa×s	617.57	Joback Method
dvisc	0.0001630	Pa×s	563.48	Joback Method
dvisc	0.0002518	Pa×s	509.40	Joback Method
dvisc	0.0004315	Pa×s	455.31	Joback Method
dvisc	0.0008547	Pa×s	401.23	Joback Method
dvisc	0.0020950	Pa×s	347.14	Joback Method

Sources

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=R399485&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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