o-Homoveratric acid

Other names: Acetic acid, (2,3-dimethoxyphenyl)-
Benzeneacetic acid, 2,3-dimethoxy-
2,3-Dimethoxyphenylacetic acid
Inchi: InChI=1S/C10H12O4/c1-13-8-5-3-4-7(6-9(11)12)10(8)14-2/h3-5H,6H2,1-2H3,(H,11,12)
InchiKey: UZULEJNWMHZSGY-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: COc1cccc(CC(=O)O)c1OC
Mol. weight [g/mol]: 196.20
CAS: 90-53-9

Physical Properties

Property code	Value	Unit	Source
gf	-349.27	kJ/mol	Joback Method
hf	-565.39	kJ/mol	Joback Method
hfus	22.98	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.331		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	655.73	K	Joback Method
tc	854.45	K	Joback Method
tf	409.13	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.72	J/mol×K	655.73	Joback Method
cpg	420.44	J/mol×K	821.33	Joback Method
cpg	412.05	J/mol×K	788.21	Joback Method
cpg	403.09	J/mol×K	755.09	Joback Method
cpg	393.54	J/mol×K	721.97	Joback Method
cpg	383.42	J/mol×K	688.85	Joback Method

cpg	428.23	J/mol×K	854.45	Joback Method
dvisc	0.0000485	Pa×s	655.73	Joback Method
dvisc	0.0000685	Pa×s	614.63	Joback Method
dvisc	0.0001017	Pa×s	573.53	Joback Method
dvisc	0.0001606	Pa×s	532.43	Joback Method
dvisc	0.0002737	Pa×s	491.33	Joback Method
dvisc	0.0005142	Pa×s	450.23	Joback Method
dvisc	0.0010962	Pa×s	409.13	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=C90539&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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