3,5-Dimethoxy-4-hydroxyphenylacetic acid

Other names:	Homosyringic acid
	Benzeneacetic acid, 4-hydroxy-3,5-dimethoxy-
	4-hydroxy-3,5-dimethoxyphenylacetic acid
Inchi:	InChI=1S/C10H12O5/c1-14-7-3-6(5-9(11)12)4-8(15-2)10(7)13/h3-4,13H,5H2,1-2H3,(H,1
InchiKey:	BQBQKSSTFGCRQL-UHFFFAOYSA-N
Formula:	C10H12O5
SMILES:	COc1cc(CC(=O)O)cc(OC)c1O
Mol. weight [g/mol]:	212.20
CAS:	4385-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-503.89	kJ/mol	Joback Method
hf	-742.70	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	82.71	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.036		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	736.35	K	Joback Method
tc	944.15	K	Joback Method
tf	520.85	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.81	J/mol×K	736.35	Joback Method
cpg	459.63	J/mol×K	909.52	Joback Method
cpg	451.98	J/mol×K	874.89	Joback Method
cpg	443.91	J/mol×K	840.25	Joback Method
cpg	435.37	J/mol×K	805.62	Joback Method
cpg	426.35	J/mol×K	770.98	Joback Method

cpg	466.86	J/mol×K	944.15	Joback Method
dvisc	0.0000030	Pa×s	736.35	Joback Method
dvisc	0.0000046	Pa×s	700.43	Joback Method
dvisc	0.0000072	Pa×s	664.52	Joback Method
dvisc	0.0000119	Pa×s	628.60	Joback Method
dvisc	0.0000211	Pa×s	592.68	Joback Method
dvisc	0.0000401	Pa×s	556.77	Joback Method
dvisc	0.0000834	Pa×s	520.85	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=C4385562&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume