

3,5-Dimethoxyphenylacetic acid

Other names:	Benzeneacetic acid, 3,5-dimethoxy-
Inchi:	InChI=1S/C10H12O4/c1-13-8-3-7(5-10(11)12)4-9(6-8)14-2/h3-4,6H,5H2,1-2H3,(H,11,12)
InchiKey:	FFPAFDDLAGTG PQ-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COc1cc(CC(=O)O)cc(OC)c1
Mol. weight [g/mol]:	196.20
CAS:	4670-10-4

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.72	J/molxK	655.73	Joback Method
cpg	420.44	J/molxK	821.33	Joback Method
cpg	412.05	J/molxK	788.21	Joback Method
cpg	403.09	J/molxK	755.09	Joback Method
cpg	393.54	J/molxK	721.97	Joback Method
cpg	383.42	J/molxK	688.85	Joback Method
cpg	428.23	J/molxK	854.45	Joback Method
dvisc	0.0000485	Paxs	655.73	Joback Method

dvisc	0.0000685	Paxs	614.63	Joback Method
dvisc	0.0001017	Paxs	573.53	Joback Method
dvisc	0.0001606	Paxs	532.43	Joback Method
dvisc	0.0002737	Paxs	491.33	Joback Method
dvisc	0.0005142	Paxs	450.23	Joback Method
dvisc	0.0010962	Paxs	409.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4670104&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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