

3,4,5-Trimethoxyphenylacetic acid

Other names:	Benzeneacetic acid, 3,4,5-trimethoxy-
Inchi:	InChI=1S/C11H14O5/c1-14-8-4-7(6-10(12)13)5-9(15-2)11(8)16-3/h4-5H,6H2,1-3H3,(H,1
InchiKey:	DDSJXCGGOXKGSJ-UHFFFAOYSA-N
Formula:	C11H14O5
SMILES:	COc1cc(CC(=O)O)cc(OC)c1OC
Mol. weight [g/mol]:	226.23
CAS:	951-82-6

Physical Properties

Property code	Value	Unit	Source
gf	-455.48	kJ/mol	Joback Method
hf	-729.72	kJ/mol	Joback Method
hfus	26.37	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.339		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	706.01	K	Joback Method
tc	902.24	K	Joback Method
tf	455.15	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.85	J/molxK	706.01	Joback Method
cpg	495.31	J/molxK	869.54	Joback Method
cpg	486.74	J/molxK	836.83	Joback Method
cpg	477.48	J/molxK	804.13	Joback Method
cpg	467.57	J/molxK	771.42	Joback Method
cpg	457.02	J/molxK	738.72	Joback Method
cpg	503.19	J/molxK	902.24	Joback Method
dvisc	0.0000299	Paxs	706.01	Joback Method

dvisc	0.0000410	Paxs	664.20	Joback Method
dvisc	0.0000588	Paxs	622.39	Joback Method
dvisc	0.0000888	Paxs	580.58	Joback Method
dvisc	0.0001428	Paxs	538.77	Joback Method
dvisc	0.0002490	Paxs	496.96	Joback Method
dvisc	0.0004806	Paxs	455.15	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=C951826&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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