3-(3,4,5-TRIMETHOXYPHENYL)PROPIONIC ACID

Other names: 3,4,5-Trimethoxyphenylpropionic acid
3,4,5-trimethoxyhydrocinnamic acid
3-(3,4,5-Trimethoxyphenyl)propanoic acid
Benzenepropanoic acid, 3,4,5-trimethoxy-
«beta»-(3,4,5-Trimethoxy phenyl)propionic acid

Inchi: InChI=1S/C12H16O5/c1-15-9-6-8(4-5-11(13)14)7-10(16-2)12(9)17-3/h6-7H,4-5H2,1-3H3

InchiKey: ZCYXGVJUZBKJAI-UHFFFAOYSA-N

Formula: C12H16O5

SMILES: COc1cc(CCC(=O)O)cc(OC)c1OC

Mol. weight [g/mol]: 240.26

Physical Properties

Property code	Value	Unit	Source
hfus	28.96	kJ/mol	Joback Method
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)
logp	1.730		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	601.83	K	Cheméo Relay (1.0)
tf	401.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.77	J/mol×K	728.89	Joback Method
cpg	509.53	J/mol×K	761.35	Joback Method
cpg	520.60	J/mol×K	793.81	Joback Method
cpg	530.98	J/mol×K	826.26	Joback Method
cpg	540.64	J/mol×K	858.72	Joback Method
cpg	549.57	J/mol×K	891.18	Joback Method
cpg	557.76	J/mol×K	923.64	Joback Method
dvisc	0.0004238	Pa×s	466.42	Joback Method
dvisc	0.0002165	Pa×s	510.16	Joback Method

dvisc	0.0001230	Pa×s	553.91	Joback Method
dvisc	0.0000759	Pa×s	597.65	Joback Method
dvisc	0.0000501	Pa×s	641.40	Joback Method
dvisc	0.0000348	Pa×s	685.14	Joback Method
dvisc	0.0000253	Pa×s	728.89	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25173722&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point