3-(3,4,5-Trimethoxyphenyl)propionic acid

Other names: 3-(3,4,5-Trimethoxyphenyl)propanoic acid
3,4,5-Trimethoxyphenylpropionic acid
«beta»-(3,4,5-Trimethoxy phenyl)propionic acid
Benzenepropanoic acid, 3,4,5-trimethoxy-
3,4,5-trimethoxyhydrocinnamic 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]: 240.25
CAS: 25173-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-447.06	kJ/mol	Joback Method
hf	-750.36	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.730		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	728.89	K	Joback Method
tc	923.64	K	Joback Method
tf	466.42	K	Joback Method
vc	0.678	m3/kmol	Joback Method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25173722&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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