

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

<b>Other names:</b>	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
<b>Inchi:</b>	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
<b>InchiKey:</b>	ZCYXGVJUJBKJAI-UHFFFAOYSA-N
<b>Formula:</b>	C12H16O5
<b>SMILES:</b>	COc1cc(CCC(=O)O)cc(OC)c1OC
<b>Mol. weight [g/mol]:</b>	240.25
<b>CAS:</b>	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/molxK	728.89	Joback Method
cpg	509.53	J/molxK	761.35	Joback Method
cpg	520.60	J/molxK	793.81	Joback Method
cpg	530.98	J/molxK	826.26	Joback Method

cpg	540.64	J/molxK	858.72	Joback Method
cpg	549.57	J/molxK	891.18	Joback Method
cpg	557.76	J/molxK	923.64	Joback Method
dvisc	0.0004238	Paxs	466.42	Joback Method
dvisc	0.0002165	Paxs	510.16	Joback Method
dvisc	0.0001230	Paxs	553.91	Joback Method
dvisc	0.0000759	Paxs	597.65	Joback Method
dvisc	0.0000501	Paxs	641.40	Joback Method
dvisc	0.0000348	Paxs	685.14	Joback Method
dvisc	0.0000253	Paxs	728.89	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25173722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25173722&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/85-246-5/3-3-4-5-Trimethoxyphenyl-propionic-acid.pdf>

Generated by Cheméo on 2025-12-23 02:35:25.787979386 +0000 UTC m=+6205523.318020050.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.