

# Benzeneethanamine,2,4,5-trimethoxy-«alpha»-me

<b>Inchi:</b>	InChI=1S/C12H19NO3/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-8H,5,13H2,1-4H3
<b>InchiKey:</b>	TVSIMAWGATVNGK-UHFFFAOYSA-N
<b>Formula:</b>	C12H19NO3
<b>SMILES:</b>	COc1cc(OC)c(OC)cc1CC(C)N
<b>Mol. weight [g/mol]:</b>	225.28
<b>CAS:</b>	22199-15-1

## Physical Properties

Property code	Value	Unit	Source
gf	-117.31	kJ/mol	Joback Method
hf	-457.04	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
ie	7.66	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
ie	7.66 ± 0.06	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	1.602		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	654.93	K	Joback Method
tc	864.02	K	Joback Method
tf	423.93	K	Joback Method
vc	0.676	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.94	J/molxK	654.93	Joback Method
cpg	504.12	J/molxK	689.78	Joback Method
cpg	518.51	J/molxK	724.63	Joback Method
cpg	532.11	J/molxK	759.48	Joback Method
cpg	544.90	J/molxK	794.33	Joback Method
cpg	556.85	J/molxK	829.17	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=C22199151&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22199151&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>ie:</b>	Ionization energy
<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

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