

# Benzeneethanamine, 3,4,5-trimethoxy-

<b>Other names:</b>	Phenethylamine, 3,4,5-trimethoxy- Mescaline Mezcalin Mezcaline TMPEA 3,4,5-Trimethoxyphenethylamine 3,4,5-Trimethoxyphenylethylamine Ethane, 1-amino-2-(3,4,5-trimethoxyphenyl)- Mescline Mezcline 3,4,5-Trimethoxybenzeneethanamine Mescaline 2-(3,4,5-Trimethoxyphenyl)ethylamine NSC 30419
<b>Inchi:</b>	InChI=1S/C11H17NO3/c1-13-9-6-8(4-5-12)7-10(14-2)11(9)15-3/h6-7H,4-5,12H2,1-3H3
<b>InchiKey:</b>	RHCSKNNOAZULRK-UHFFFAOYSA-N
<b>Formula:</b>	C11H17NO3
<b>SMILES:</b>	COc1cc(CCN)cc(OC)c1OC
<b>Mol. weight [g/mol]:</b>	211.26
<b>CAS:</b>	54-04-6

## Physical Properties

Property code	Value	Unit	Source
gf	-123.29	kJ/mol	Joback Method
hf	-431.12	kJ/mol	Joback Method
hfus	25.88	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
ie	8.18 ± 0.24	eV	NIST Webbook
log10ws	-2.07		Crippen Method
logp	1.214		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1663.00		NIST Webbook

rinpol	1663.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	632.49	K	Joback Method
tc	840.81	K	Joback Method
tf	427.66	K	Joback Method
vc	0.626	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.68	J/molxK	632.49	Joback Method
cpg	451.89	J/molxK	667.21	Joback Method
cpg	465.41	J/molxK	701.93	Joback Method
cpg	478.24	J/molxK	736.65	Joback Method
cpg	490.35	J/molxK	771.37	Joback Method
cpg	501.72	J/molxK	806.09	Joback Method
cpg	512.33	J/molxK	840.81	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	1.60	NIST Webbook

# Sources

<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=C54046&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54046&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>
<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>

# 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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