Benzeneethanamine, 3,4,5-trimethoxy-

Other names:	Phenethylamine, 3,4,5-trimethoxy-
	Mescalin
	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
Inchi:	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
InchiKey:	RHCSKNNOAZULRK-UHFFFAOYSA-N
Formula:	C11H17NO3
SMILES:	COc1cc(CCN)cc(OC)c1OC
Mol. weight [g/mol]:	211.26
CAS:	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	1695.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1664.00		NIST Webbook

rinpol	1688.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1663.00		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	1731.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	632.49	K	Joback Method
tc	840.81	K	Joback Method
tf	427.66	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54046&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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume