Benzeneethanamine,3,4,5-trimethoxy-N-methyl-

Other names:	Benzenethanamine,3,4,5-trimethoxy-N-methyl- Mescaline, N-methyl- N-Methylmescaline
Inchi:	InChI=1S/C12H19NO3/c1-13-6-5-9-7-10(14-2)12(16-4)11(8-9)15-3/h7-8,13H,5-6H2,1-4H
InchiKey:	OTXANOLOOUNVSR-UHFFFAOYSA-N
Formula:	C12H19NO3
SMILES:	CNCCc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]:	225.28
CAS:	4838-96-4

Physical Properties

Property code	Value	Unit	Source
gf	-91.93	kJ/mol	Joback Method
hf	-432.08	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.474		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1700.00		NIST Webbook
tb	633.01	K	Joback Method
tc	831.08	K	Joback Method
tf	408.33	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.50	J/mol×K	633.01	Joback Method
cpg	492.54	J/mol×K	666.02	Joback Method
cpg	506.89	J/mol×K	699.03	Joback Method
cpg	520.53	J/mol×K	732.04	Joback Method
cpg	533.45	J/mol×K	765.05	Joback Method

cpg	545.63	J/mol×K	798.07	Joback Method
cpg	557.06	J/mol×K	831.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4838964&Units=SI

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/18-855-3/Benzeneethanamine-3-4-5-trimethoxy-N-methyl.pdf
Generated by Cheméo on 2024-10-12 06:12:36.016240009 +0000 UTC m=+3294418.653209257.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.