

Benzeneethanamine, N,«alpha»,«alpha»-trimethyl-

Other names:

Phenethylamine, N,«alpha»,«alpha»-trimethyl-
«omega»-Phenyl-tert-butyl-methylamine
Mephine
N,«alpha»,«alpha»-Trimethyl-«beta»-phenethylamine
N,«alpha»,«alpha»-Trimethylphenethylamine
Vialin
Wyamine
Mefenterdrin
Mefentermin
Mephenterdrine
Mephenterdrinum
Mephedrine
2-Methylamino-2-methyl-1-phenylpropane
2-Methyl-2-methylamino-1-phenylpropane
N-Methyl-«omega»-phenyl-t-butylamine
N,«alpha»,«alpha»-Trimethylbenzeneethanamine
WY-585
Wyfentermina
N-Methyl-«omega»-phenyl-tert-butylamine
N-Methylphentermine
Mephentermine
InChI=1S/C11H17N/c1-11(2,12-3)9-10-7-5-4-6-8-10/h4-8,12H,9H2,1-3H3
RXQCGGRTAILOIN-UHFFFAOYSA-N
C11H17N
CNC(C)(C)Cc1cccc1
163.26
100-92-5

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

Physical Properties

Property code	Value	Unit	Source
gf	246.38	kJ/mol	Joback Method
hf	10.88	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.227		Crippen Method

mcvol	152.070	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1236.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1611.00		NIST Webbook
tb	524.70	K	Joback Method
tc	741.06	K	Joback Method
tf	295.23	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.65	J/mol×K	524.70	Joback Method
cpg	370.82	J/mol×K	560.76	Joback Method
cpg	386.85	J/mol×K	596.82	Joback Method
cpg	401.78	J/mol×K	632.88	Joback Method
cpg	415.69	J/mol×K	668.94	Joback Method
cpg	428.64	J/mol×K	705.00	Joback Method
cpg	440.70	J/mol×K	741.06	Joback Method

Sources

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=C100925&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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