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

Other names:	Phenethylamine, N,N,«alpha»-trimethyl-
	Dimethylamphetamine
	N,N,«alpha»-Trimethylphenethylamine
	2-Dimethylamino-1-phenylpropane
	1-Phenyl-2-dimethylamino-propan
	«alpha»-Phenyl-«beta»-dimethylaminopropane
	1-Phenyl-2-dimethylaminopropane
	N,N-Dimethylamphetamine
Inchi:	InChI=1S/C11H17N/c1-10(12(2)3)9-11-7-5-4-6-8-11/h4-8,10H,9H2,1-3H3
InchiKey:	OBDSVYOSYSKVMX-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CC(Cc1ccccc1)N(C)C
Mol. weight [g/mol]:	163.26
CAS:	4075-96-1

Physical Properties

Property code	Value	Unit	Source
gf	262.49	kJ/mol	Joback Method
hf	28.41	kJ/mol	Joback Method
hfus	17.79	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.179		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1236.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	489.76	K	Joback Method
tc	693.60	K	Joback Method
tf	257.62	K	Joback Method

vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.54	J/mol×K	489.76	Joback Method
cpg	350.82	J/mol×K	523.73	Joback Method
cpg	367.10	J/mol×K	557.71	Joback Method
cpg	382.41	J/mol×K	591.68	Joback Method
cpg	396.81	J/mol×K	625.65	Joback Method
cpg	410.33	J/mol×K	659.62	Joback Method
cpg	423.02	J/mol×K	693.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4075961&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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