

Tricyclo[3.3.1.1^{3,7}]decan-1-amine, N,N-dimethyl-

Other names:	(Dimethylamino)adamantane N,N-Dimethyl-1-adamantylamine 1-(Dimethylamino)adamantane N,N-Dimethyl-1-adamantanamine Tricyclo(3.3.1.1
Inchi:	InChI=1S/C12H21N/c1-13(2)12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11H,3-8H2,1-2H3
InchiKey:	NFBYCNFAXLUGBT-UHFFFAOYSA-N
Formula:	C12H21N
SMILES:	CN(C)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	179.31

Physical Properties

Property code	Value	Unit	Source
affp	993.90	kJ/mol	NIST Webbook
basg	963.00	kJ/mol	NIST Webbook
hf	-132.57	kJ/mol	Cheméo Relay (1.0)
hfus	16.94	kJ/mol	Joback Method
ie	7.53	eV	Cheméo Relay (1.0)
logp	2.517		Crippen Method
mcvol	157.340	ml/mol	McGowan Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1470.00		NIST Webbook
tf	472.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.93	J/mol×K	506.46	Joback Method
cpg	426.60	J/mol×K	542.03	Joback Method
cpg	447.54	J/mol×K	577.61	Joback Method
cpg	466.95	J/mol×K	613.18	Joback Method
cpg	485.00	J/mol×K	648.76	Joback Method
cpg	501.90	J/mol×K	684.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3717406&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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