

(CH3)3CCH2N(CH3)2

Other names:	N,N-Dimethyl neopentylamine Dimethyl(neopentyl)amine
Inchi:	InChI=1S/C7H17N/c1-7(2,3)6-8(4)5/h6H2,1-5H3
InchiKey:	FUIRUFXAVIHAQB-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CN(C)CC(C)(C)C
Mol. weight [g/mol]:	115.22
CAS:	10076-31-0

Physical Properties

Property code	Value	Unit	Source
affp	970.50	kJ/mol	NIST Webbook
basg	939.50	kJ/mol	NIST Webbook
gf	121.68	kJ/mol	Joback Method
hf	-129.03	kJ/mol	Joback Method
hfus	9.49	kJ/mol	Joback Method
hvap	31.92	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.594		Crippen Method
mvol	119.470	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	368.77	K	Joback Method
tc	542.09	K	Joback Method
tf	203.54	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.99	J/molxK	368.77	Joback Method
cpg	236.63	J/molxK	397.66	Joback Method
cpg	250.57	J/molxK	426.54	Joback Method
cpg	263.82	J/molxK	455.43	Joback Method
cpg	276.41	J/molxK	484.32	Joback Method

cpg	288.38	J/mol×K	513.20	Joback Method
cpg	299.74	J/mol×K	542.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C10076310&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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