

N-METHYL-TERT-BUTYLAMINE

Other names:	2-Propanamine, N,2-dimethyl- N-Methyl-tert-butylamine tert-butylmethanamine
Inchi:	InChI=1S/C5H13N/c1-5(2,3)6-4/h6H,1-4H3
InchiKey:	ZQGJEUVBUBVKZKS-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CNC(C)(C)C
Mol. weight [g/mol]:	87.17

Physical Properties

Property code	Value	Unit	Source
hfus	6.39	kJ/mol	Joback Method
ie	8.08	eV	Cheméo Relay (1.0)
logp	1.004		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
rinpol	607.00		NIST Webbook
rinpol	607.00		NIST Webbook
tb	346.65 ± 1.50	K	NIST Webbook
tb	332.15 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.44	J/mol×K	360.74	Joback Method
cpg	175.08	J/mol×K	391.06	Joback Method
cpg	186.14	J/mol×K	421.37	Joback Method
cpg	196.65	J/mol×K	451.69	Joback Method
cpg	206.62	J/mol×K	482.01	Joback Method
cpg	216.07	J/mol×K	512.33	Joback Method
cpg	225.03	J/mol×K	542.64	Joback Method
hvapt	32.30 ± 1.40	kJ/mol	279.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C14610378&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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