

1-BUTANAMINE, 3-METHYL-N-(3-METHYLBUTYLIDENE)-

Other names:	3-Methyl-N-(3-methylbutylidene)-1-butanamine 3-Methyl-N-(3'-methylbutylidene)butanamine 3-Methyl-N-(3-methylbutylidene)-butanamine Butanamine, 3-methyl-N-(3-methylbutylidene) N-Isopentylidene isopentylamine 3-methyl-N-(3-methylbutyl)butan-1-imine
Inchi:	InChI=1S/C10H21N/c1-9(2)5-7-11-8-6-10(3)4/h7,9-10H,5-6,8H2,1-4H3
InchiKey:	WYNULUURQZBBSK-UHFFFAOYSA-N
Formula:	C10H21N
SMILES:	<chem>CC(C)CC=NCCC(C)C</chem>
Mol. weight [g/mol]:	155.29

Physical Properties

Property code	Value	Unit	Source
logp	3.149		Crippen Method
mcvol	157.440	ml/mol	McGowan Method
rinpol	1033.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1033.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1130.00		NIST Webbook

Sources

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):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C35448318&Units=SI>

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

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