

Isobutyl azide

Inchi: InChI=1S/C4H11N3/c1-4(2)3-6-7-5/h4-5,7H,3H2,1-2H3
InchiKey: KXEHHYUNOXDITF-UHFFFAOYSA-N
Formula: C4H11N3
SMILES: CC(C)C[N]N[NH]
Mol. weight [g/mol]: 101.15

Physical Properties

Property code	Value	Unit	Source
log10ws	9.48		Crippen Method
logp	-0.051		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
rinpola	719.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R511858&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/55-013-6/Isobutyl-azide.pdf>

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