

2-n-butyl-6-methylpyridine

Inchi: InChI=1S/C10H15N/c1-3-4-7-10-8-5-6-9(2)11-10/h5-6,8H,3-4,7H2,1-2H3
InchiKey: CTIJGOMYLLUVIK-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CCCCC1CCCC(C)N1
Mol. weight [g/mol]: 149.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.733		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
ripol	1485.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1485.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R296841&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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<https://www.chemeo.com/cid/76-393-2/2-n-butyl-6-methylpyridine.pdf>

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