2-Isobutyl-4-methylpyridine

Inchi:	InChI=1S/C10H15N/c1-8(2)6-10-7-9(3)4-5-11-10/h4-5,7-8H,6H2,1-3H3
InchiKey:	GZUWMFOJIYTMTM-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	Cc1ccnc(CC(C)C)c1
Mol. weight [g/mol]:	149.23
CAS:	85665-88-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	2.589		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
rinpol	1154.00		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=C85665889&Units=SI

Legend

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

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