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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.