

2,5-diethylpyridine

Inchi: InChI=1S/C9H13N/c1-3-8-5-6-9(4-2)10-7-8/h5-7H,3-4H2,1-2H3
InchiKey: IXFAHCCRDS SCPX-UHFFFAOYSA-N
Formula: C9H13N
SMILES: CCc1ccc(CC)nc1
Mol. weight [g/mol]: 135.21
CAS: 54119-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.206		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpola	1422.00		NIST Webbook
rinpola	1422.00		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=C54119298&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/47-077-5/2-5-diethylpyridine.pdf>

Generated by Cheméo on 2024-04-19 20:42:51.886533805 +0000 UTC m=+15848620.807111165.

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