

1-(3-Pyridyl)-2-(4-pyridyl)ethylene

Inchi: InChI=1S/C12H10N2/c1-2-12(10-14-7-1)4-3-11-5-8-13-9-6-11/h1-10H/b4-3+
InchiKey: LELJBILQTLAIMQ-ONEGZZNKSA-N
Formula: C12H10N2
SMILES: C(=Cc1ccnc1)c1ccncc1
Mol. weight [g/mol]: 182.22
CAS: 2682-93-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.647		Crippen Method
mcvol	148.080	ml/mol	McGowan Method
rinpol	1936.00		NIST Webbook
rinpol	1936.00		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=C2682931&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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<https://www.chemeo.com/cid/65-119-8/1-3-Pyridyl-2-4-pyridyl-ethylene.pdf>

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