

Pyridine, 3,5-di(4-methylphenyl)-

Inchi: InChI=1S/C19H17N/c1-14-3-7-16(8-4-14)18-11-19(13-20-12-18)17-9-5-15(2)6-10-17/h3-
InchiKey: KKFPMNGOXKYTRG-UHFFFAOYSA-N
Formula: C19H17N
SMILES: Cc1ccc(-c2cncc(-c3ccc(C)cc3)c2)cc1
Mol. weight [g/mol]: 259.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.39		Crippen Method
logp	5.032		Crippen Method
mcvol	217.270	ml/mol	McGowan Method
rinpola	2616.00		NIST Webbook
rinpola	2616.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U380548&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

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