

Pyridazine, 3,6-di(4-methylphenyl)-

Inchi: InChI=1S/C18H16N2/c1-13-3-7-15(8-4-13)17-11-12-18(20-19-17)16-9-5-14(2)6-10-16/h3
InchiKey: WVNRLKLGKGNMYAQ-UHFFFAOYSA-N
Formula: C18H16N2
SMILES: Cc1ccc(-c2ccc(-c3ccc(C)cc3)nn2)cc1
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	4.427		Crippen Method
mcvol	213.160	ml/mol	McGowan Method
rinpol	2939.00		NIST Webbook
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Sources

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=U380556&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/81-787-9/Pyridazine-3-6-di-4-methylphenyl.pdf>

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