

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

Inchi: InChI=1S/C11H9ClN2/c1-8-2-4-9(5-3-8)10-6-7-11(12)14-13-10/h2-7H,1H3
InchiKey: MCDSGZGKYCPLMT-UHFFFAOYSA-N
Formula: C11H9ClN2
SMILES: Cc1ccc(-c2ccc(Cl)nn2)cc1
Mol. weight [g/mol]: 204.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.105		Crippen Method
mcvol	150.530	ml/mol	McGowan Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		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=U380555&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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