

3,6-dimethylpyridazine

Inchi: InChI=1S/C6H8N2/c1-5-3-4-6(2)8-7-5/h3-4H,1-2H3
InchiKey: BGVUIRPHLSMJU-UHFFFAOYSA-N
Formula: C6H8N2
SMILES: Cc1ccc(C)nn1
Mol. weight [g/mol]: 108.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.093		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R193816&Units=SI>
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>

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/50-330-9/3-6-dimethylpyridazine.pdf>

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