Pyrimidine, 5-(4-methylphenyl)-

Inchi: InChI=1S/C11H10N2/c1-9-2-4-10(5-3-9)11-6-12-8-13-7-11/h2-8H,1H3
InchiKey: HMIDRMDGUSXDTP-UHFFFAOYSA-N
Formula: C11H10N2
SMILES: Cc1ccc(-c2cncnc2)cc1
Mol. weight [g/mol]: 170.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	2.452		Crippen Method
mcvol	138.290	ml/mol	McGowan Method
rinpol	1649.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380550&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