

2,3,5-trimethyl-5,7-dihydro-(5H)-cyclopentapyrazine

Inchi: InChI=1S/C10H14N2/c1-6-4-5-9-10(6)12-8(3)7(2)11-9/h6H,4-5H2,1-3H3
InchiKey: YVBOGCYLFHKRRQ-UHFFFAOYSA-N
Formula: C10H14N2
SMILES: Cc1nc2c(nc1C)C(C)CC2
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.143		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R236567&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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<https://www.chemeo.com/cid/85-673-1/2-3-5-trimethyl-5-7-dihydro-5H-cyclopentapyrazine.pdf>

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