2,3-diethyl-5,6-dimethylpyrazine

Inchi: InChI=1S/C10H16N2/c1-5-9-10(6-2)12-8(4)7(3)11-9/h5-6H2,1-4H3
InchiKey: YAGSHZPMYHTMPZ-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCc1nc(C)c(C)nc1CC
Mol. weight [g/mol]: 164.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.218		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
ripol	1527.00		NIST Webbook
ripol	1547.00		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=R296732&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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