2-methyl-3,5-diisobutylpyrazine

Inchi: InChI=1S/C13H22N2/c1-9(2)6-12-8-14-11(5)13(15-12)7-10(3)4/h8-10H,6-7H2,1-5H3
InchiKey: HWSKHSMKHGRVBS-UHFFFAOYSA-N
Formula: C13H22N2
SMILES: Cc1ncc(CC(C)C)nc1CC(C)C
Mol. weight [g/mol]: 206.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	3.182		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
ripol	1670.00		NIST Webbook
ripol	1670.00		NIST Webbook

Sources

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=R314815&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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