

2-methyl-6-isopropylpyrazine

Inchi: InChI=1S/C8H12N2/c1-6(2)8-5-9-4-7(3)10-8/h4-6H,1-3H3
InchiKey: QSLRSJBWLFFNIS-UHFFFAOYSA-N
Formula: C8H12N2
SMILES: Cc1cncc(C(C)C)n1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	1.908		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1050.00		NIST Webbook
ripol	1387.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R325989&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
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/12-714-5/2-methyl-6-isopropylpyrazine.pdf>

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