

2-chloro-3-methyl-5-(2-methylpentyl)pyrazine

Other names: Pyrazine, 2-chloro-3-methyl-5-(2-methylpentyl)
Inchi: InChI=1S/C11H17ClN2/c1-4-5-8(2)6-10-7-13-11(12)9(3)14-10/h7-8H,4-6H2,1-3H3
InchiKey: YOZRPCPCVYSOEH-UHFFFAOYSA-N
Formula: C11H17ClN2
SMILES: CCCC(C)Cc1cnc(Cl)c(C)n1
Mol. weight [g/mol]: 212.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	3.417		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rinpol	1456.00		NIST Webbook
ripol	1789.00		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=R38288&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

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