Pyrazine, 2,3-dimethyl-5-(2-methylbutyl)

Other names: 2,3-dimethyl-5-(2-methylbutyl)pyrazine
Inchi: InChI=1S/C11H18N2/c1-5-8(2)6-11-7-12-9(3)10(4)13-11/h7-8H,5-6H2,1-4H3
InchiKey: QJQUDEDFDDMKGC-UHFFFAOYSA-N
Formula: C11H18N2
SMILES: CCC(C)Cc1cnc(C)c(C)n1
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.682		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1306.00		NIST Webbook
ripol	1636.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38210&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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