

(2-methylbutyl)pyrazine

Other names: Pyrazine, (2-methylbutyl)
Inchi: InChI=1S/C9H14N2/c1-3-8(2)6-9-7-10-4-5-11-9/h4-5,7-8H,3,6H2,1-2H3
InchiKey: WONHREJRLMEWSC-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: CCC(C)Cc1cnccn1
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.065		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
ripol	1527.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R36369&Units=SI>
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>

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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