

butyl pyrazine

Other names: Pyrazine, butyl
Inchi: InChI=1S/C8H12N2/c1-2-3-4-8-7-9-5-6-10-8/h5-7H,2-4H2,1H3
InchiKey: TVAVRPSANVGCNH-UHFFFAOYSA-N
Formula: C8H12N2
SMILES: CCCCC1CNCCN1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.819		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
ripol	1474.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R36373&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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