2-Butyl-3-methylpyrazine

Other names: 2-n-Butyl-3-methylpyrazine
Pyrazine, 2-butyl-3-methyl-
2-Methyl-3- butylpyrazine
Inchi: InChI=1S/C9H14N2/c1-3-4-5-9-8(2)10-6-7-11-9/h6-7H,3-5H2,1-2H3
InchiKey: IRSIKJPEFMMRHD-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: CCCCc1nccnc1C
Mol. weight [g/mol]: 150.22
CAS: 15987-00-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.128		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1125.00		NIST Webbook
rinpol	1121.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1459.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15987005&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