

1-methylbutylpyrazine

Other names:	sec-pentylpyrazine Pyrazine, (1-methylbutyl)
Inchi:	InChI=1S/C9H14N2/c1-3-4-8(2)9-7-10-5-6-11-9/h5-8H,3-4H2,1-2H3
InchiKey:	MRGPJALDSXTAJS-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCCC(C)c1cnccn1
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.380		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1148.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1471.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R36355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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