

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/ci990307I
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

Latest version available from:

<https://www.cheméo.com/cid/43-723-1/2-Butyl-3-methylpyrazine.pdf>

Generated by Cheméo on 2024-04-26 04:03:18.736750616 +0000 UTC m=+16393447.657327927.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.