

2-methoxy-3-butyl pyrazine

Other names:	Pyrazine, 2-butyl-3-methoxy Pyrazine, 3-butyl-2-methoxy
Inchi:	InChI=1S/C9H14N2O/c1-3-4-5-8-9(12-2)11-7-6-10-8/h6-7H,3-5H2,1-2H3
InchiKey:	CPYHBHYOFYVTEV-UHFFFAOYSA-N
Formula:	C9H14N2O
SMILES:	CCCCc1nccnc1OC
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	1.828		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1219.00		NIST Webbook
rinpol	1219.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1575.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R43613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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