

5-sec-butyl-2-ethylthio-3-methylpyrazine

Other names:	Pyrazine, 2-(ethylthio)-3-methyl-5-(1-methylpropyl)
Inchi:	InChI=1S/C11H18N2S/c1-5-8(3)10-7-12-11(14-6-2)9(4)13-10/h7-8H,5-6H2,1-4H3
InchiKey:	RJNDCTKDPDQBEN-UHFFFAOYSA-N
Formula:	C11H18N2S
SMILES:	CCSc1ncc(C(C)CC)nc1C
Mol. weight [g/mol]:	210.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.411		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
rinpol	1494.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1832.00		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=R38701&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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