

3-methyl-5-ethyl-2-isobutylpyrazine

Inchi:	InChI=1S/C11H18N2/c1-5-10-7-12-11(6-8(2)3)9(4)13-10/h7-8H,5-6H2,1-4H3
InchiKey:	NSUZNJBCWAYJHZ-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CCc1cnc(CC(C)C)c(C)n1
Mol. weight [g/mol]:	178.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.546		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
ripol	1570.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R314820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
ripol:	Polar retention indices

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