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/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
ripol: Polar retention indices