

Pyrazine, 2-ethoxy-3-methyl-5-(2-methylpentyl)

Inchi: InChI=1S/C13H22N2O/c1-5-7-10(3)8-12-9-14-13(16-6-2)11(4)15-12/h9-10H,5-8H2,1-4H
InchiKey: VBKZIEKIZTVOGB-UHFFFAOYSA-N
Formula: C13H22N2O
SMILES: CCCC(C)Cc1cnc(OCC)c(C)n1
Mol. weight [g/mol]: 222.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.162		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
ripol	1771.00		NIST Webbook
ripol	1771.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R217551&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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