Pyrazine, 2-ethoxy-3-methyl-5-(1-methylethyl)

Other names: 2-Ethoxy-5-isopropyl-3-methylpyrazine
Inchi: InChI=1S/C10H16N2O/c1-5-13-10-8(4)12-9(6-11-10)7(2)3/h6-7H,5H2,1-4H3
InchiKey: DKHOUPCRCLQJMB-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: CCOc1ncc(C(C)C)nc1C
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.307		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38331&Units=SI

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