5-sec-butyl-3-methyl-2-phenoxypyrazine

Other names: Pyrazine, 3-methyl-5-(1-methylpropyl)-2-phenoxy
Inchi: InChI=1S/C15H18N2O/c1-4-11(2)14-10-16-15(12(3)17-14)18-13-8-6-5-7-9-13/h5-11H,4H
InchiKey: DLOHAQPSNHYVHV-UHFFFAOYSA-N
Formula: C15H18N2O
SMILES: CCC(C)c1cnc(Oc2ccccc2)c(C)n1
Mol. weight [g/mol]: 242.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	4.091		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2173.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38733&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
rinpol: Non-polar retention indices
ripol: Polar retention indices