2-N-n-butylanilino-3-methyl pyrazine

Inchi: InChI=1S/C15H19N3/c1-3-4-12-18(14-8-6-5-7-9-14)15-13(2)16-10-11-17-15/h5-11H,3-4,
InchiKey: DVHOOXHYNWNOQR-UHFFFAOYSA-N
Formula: C15H19N3
SMILES: CCCCN(c1ccccc1)c1nccnc1C
Mol. weight [g/mol]: 241.33
CAS: 116660-45-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.723		Crippen Method
mcvol	204.630	ml/mol	McGowan Method

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=C116660458&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume