

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

Latest version available from:

<https://www.chemeo.com/cid/61-887-0/2-N-n-butylanilino-3-methyl-pyrazine.pdf>

Generated by Cheméo on 2025-12-22 13:09:01.791802608 +0000 UTC m=+6157139.321843261.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.