

3-(N-methylanilino)-2-(n-pentyl)-5-(n-heptyl)pyrazine

Inchi:	InChI=1S/C23H35N3/c1-4-6-8-9-12-15-20-19-24-22(18-11-7-5-2)23(25-20)26(3)21-16-13
InchiKey:	QFNYGBRCCGYZQK-UHFFFAOYSA-N
Formula:	C23H35N3
SMILES:	CCCCCCCCc1cnc(CCCCC)c(N(C)c2cccc2)n1
Mol. weight [g/mol]:	353.54
CAS:	116402-85-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	6.490		Crippen Method
mcvol	317.350	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402858&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

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