

2-(N,n-di-n-pentylamino)-3-methyl-6-(n-heptyl)pyrazine

Inchi:	InChI=1S/C22H41N3/c1-5-8-11-12-13-16-21-19-23-20(4)22(24-21)25(17-14-9-6-2)18-15
InchiKey:	XPMUGCSOHCUZDV-UHFFFAOYSA-N
Formula:	C22H41N3
SMILES:	CCCCCCCCc1cnc(C)c(N(CCCCC)CCCC)n1
Mol. weight [g/mol]:	347.58
CAS:	116402-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	6.485		Crippen Method
mcvol	327.020	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=C116402836&Units=SI

Legend

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

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