

3-(N,n-di-n-hexylamino)-2-methyl-5-(n-heptyl)-pyra

Inchi:	InChI=1S/C24H45N3/c1-5-8-11-14-15-18-23-21-25-22(4)24(26-23)27(19-16-12-9-6-2)20
InchiKey:	SNJHUPLUIRVWRZ-UHFFFAOYSA-N
Formula:	C24H45N3
SMILES:	CCCCCCCc1cnc(C)c(N(CCCCC)CCCC)n1
Mol. weight [g/mol]:	375.63
CAS:	116403-06-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.47		Crippen Method
logp	7.265		Crippen Method
mcvol	355.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116403066&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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