

2-(P-nonylphenoxy)-3-(n-pentyl)-6-(5-nonyl)pyrazine

Inchi:	InChI=1S/C33H54N2O/c1-5-9-13-14-15-16-18-19-28-23-25-30(26-24-28)36-33-31(22-17
InchiKey:	VPKTYKKCTNBEGU-UHFFFAOYSA-N
Formula:	C33H54N2O
SMILES:	CCCCCCCCCc1ccc(Oc2nc(C(CCCC)CCCC)cnc2CCCC)cc1
Mol. weight [g/mol]:	494.79
CAS:	116402-98-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.13		Crippen Method
logp	10.759		Crippen Method
mcvol	454.140	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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