

2-(P-nonylphenoxy)-6-(5-nonyl) pyrazine

Inchi:	InChI=1S/C28H44N2O/c1-4-7-10-11-12-13-14-15-24-18-20-26(21-19-24)31-28-23-29-22
InchiKey:	GWAAJIHTWWATDR-UHFFFAOYSA-N
Formula:	C28H44N2O
SMILES:	CCCCCCCCc1ccc(Oc2cncc(C(CCCC)CCCC)n2)cc1
Mol. weight [g/mol]:	424.66
CAS:	116402-93-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.07		Crippen Method
logp	9.026		Crippen Method
mcvol	383.690	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402938&Units=SI
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

Legend

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

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