

2-(2,2-Dimethylpentoxy)-3,6-di-(n-heptyl)pyrazine

Inchi:	InChI=1S/C25H46N2O/c1-6-9-11-13-15-17-22-20-26-23(18-16-14-12-10-7-2)24(27-22)25
InchiKey:	JFQDNLRHJUDZAR-UHFFFAOYSA-N
Formula:	C25H46N2O
SMILES:	CCCCCCCc1cnc(CCCCCC)c(OCC(C)(C)CCC)n1
Mol. weight [g/mol]:	390.65
CAS:	116403-03-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.18		Crippen Method
logp	7.707		Crippen Method
mcvol	365.180	ml/mol	McGowan Method

Sources

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=C116403033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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