

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

Inchi:	InChI=1S/C19H34N2O/c1-6-8-9-10-11-12-17-14-20-16(3)18(21-17)22-15-19(4,5)13-7-2/
InchiKey:	FSHSCUJFVBMKHO-UHFFFAOYSA-N
Formula:	C19H34N2O
SMILES:	CCCCCCCCc1cnc(C)c(OCC(C)(C)CCC)n1
Mol. weight [g/mol]:	306.49
CAS:	116660-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	5.503		Crippen Method
mcvol	280.640	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=C116660345&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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