

2,6-Di-(5-nonyl) pyrazine

Inchi: InChI=1S/C22H40N2/c1-5-9-13-19(14-10-6-2)21-17-23-18-22(24-21)20(15-11-7-3)16-12
InchiKey: SNVKDWFYFWFNFE-UHFFFAOYSA-N
Formula: C22H40N2
SMILES: CCCCC(CCCC)c1cncc(C(CCCC)CCCC)n1
Mol. weight [g/mol]: 332.57
CAS: 116660-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Crippen Method
logp	7.405		Crippen Method
mcvol	317.040	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660061&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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