2-(N,n-di-n-pentylamino)-3-methyl-6-(n-heptyl) pyrazine

Inchi: InChI=1S/C22H41N3/c1-5-8-11-12-13-16-21-19-23-20(4)22(24-21)25(17-14-9-6-2)18-15-

InchiKey: XPMUGCSOHCUZDV-UHFFFAOYSA-N

Formula: C22H41N3

SMILES: CCCCCCCc1cnc(C)c(N(CCCCC)CCCCC)n1

Mol. weight [g/mol]: 347.58

CAS: 116402-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	6.485		Crippen Method
mcvol	327.020	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=C116402836&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume