2-(N-n-di-n-hexylamino)-3-(n-pentyl)-6-(n-heptyl) pyrazine

Inchi: InChI=1S/C28H53N3/c1-5-9-13-16-18-21-26-25-29-27(22-17-12-8-4)28(30-26)31(23-19-

InchiKey: IZPGULQMHORVJY-UHFFFAOYSA-N

Formula: C28H53N3

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

Mol. weight [g/mol]: 431.74

CAS: 116402-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.05		Crippen Method
logp	8.689		Crippen Method
mcvol	411.560	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=C116402803&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume