4,4'-Bis(octyloxy)azoxybenzene

Inchi: InChI=1S/C28H42N2O3/c1-3-5-7-9-11-13-23-32-27-19-15-25(16-20-27)29-30(31)26-17-2
InchiKey: LMDKWWQEAJSHLR-UHFFFAOYSA-N
Formula: C28H42N2O3
SMILES: CCCCCCCCOc1ccc(N=[N+]([O-])c2ccc(OCCCCCCCC)cc2)cc1
Mol. weight [g/mol]: 454.64
CAS: 25729-12-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.50		Crippen Method
logp	9.091		Crippen Method
mcvol	391.130	ml/mol	McGowan Method
tt	353.00 ± 0.10	K	NIST Webbook
tt	380.90 ± 0.10	K	NIST Webbook
tt	399.30 ± 0.10	K	NIST Webbook

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=C25729128&Units=SI

Legend

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

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