

Diazene, bis[4-(decyloxy)phenyl]-, 1-oxide

Inchi: InChI=1S/C32H50N2O3/c1-3-5-7-9-11-13-15-17-27-36-31-23-19-29(20-24-31)33-34(35)
InchiKey: KROBVZCMTVSTEP-UHFFFAOYSA-N
Formula: C32H50N2O3
SMILES: CCCCCCCCCCOc1ccc(N=[N+](O-])c2ccc(OCCCCCCCCC)cc2)cc1
Mol. weight [g/mol]: 510.75
CAS: 2312-12-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.18		Crippen Method
logp	10.651		Crippen Method
mcvol	447.490	ml/mol	McGowan Method
tt	351.00 ± 0.10	K	NIST Webbook

Sources

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=C2312121&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/34-432-4/Diazene-bis-4-decyloxy-phenyl-1-oxide.pdf>

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