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

Other names:	4,4'-Diheptyloxyazoxybenzene
	4,4'-Bis(heptyloxy)azoxybenzene
	p-Diheptyloxyazoxybenzene
	p,p'-Diheptyloxyazoxybenzene
	Azoxybenzene, 4,4'-bis(heptyloxy)-
	4,4'-Diheptoxyazoxybenzene
	1,2-Bis[4-(heptyloxy)phenyl]diazene 1-oxide
	Diazene, 1,2-bis[4-(heptyloxy)phenyl]-, 1-oxide
	NSC 171005
	p,p'-bis(heptyloxy)azoxybenzene
Inchi:	InChI=1S/C26H38N2O3/c1-3-5-7-9-11-21-30-25-17-13-23(14-18-25)27-28(29)24-15-19-2
InchiKey:	RFRFUCJJSRXPEE-UHFFFAOYSA-N
Formula:	C26H38N2O3
SMILES:	CCCCCCCOc1ccc(N=[N+]([O-])c2ccc(OCCCCCCC)cc2)cc1
Mol. weight [g/mol]:	426.59
CAS:	2635-26-9

Physical Properties

Property code	Value	Unit	Source
ie	7.57	eV	NIST Webbook
log10ws	-8.67		Crippen Method
logp	8.311		Crippen Method
mcvol	362.950	ml/mol	McGowan Method
tt	348.00 ± 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=C2635269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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