

4,4'-Diheptylazoxybenzene

Inchi:	InChI=1S/C26H38N2O/c1-3-5-7-9-11-13-23-15-19-25(20-16-23)27-28(29)26-21-17-24(18)
InchiKey:	QGBNLWGTPRDGLR-UHFFFAOYSA-N
Formula:	C26H38N2O
SMILES:	CCCCCCCCc1ccc(N=[N+][O-])c2ccc(CCCCCC)cc2)cc1
Mol. weight [g/mol]:	394.59
CAS:	37592-89-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.20		Crippen Method
logp	8.638		Crippen Method
mcvol	351.210	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=C37592895&Units=SI

Legend

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

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<https://www.chemeo.com/cid/56-659-9/4-4-Diheptylazoxybenzene.pdf>

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