

4,4'-DIHEPTYLOXYAZOXYBENZENE

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-
InchiKey:	RFRFUCJJSRXPEE-UHFFFAOYSA-N
Formula:	C26H38N2O3
SMILES:	CCCCCCCCOc1ccc(N=[N+])([O-])c2ccc(OCCCCCCC)cc2)cc1
Mol. weight [g/mol]:	426.60

Physical Properties

Property code	Value	Unit	Source
hf	-261.11	kJ/mol	Cheméo Relay (1.0)
ie	7.57	eV	NIST Webbook
logp	8.311		Crippen Method
mcvol	362.950	ml/mol	McGowan Method
tb	718.24	K	Cheméo Relay (1.0)
tf	329.30	K	Cheméo Relay (1.0)
tt	348.00 ± 0.10	K	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2635269&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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