(4,4'-Diheptyl)azoxybenzene

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: CCCCCCCc1ccc(N=[N+]([O-])c2ccc(CCCCCCC)cc2)cc1
Mol. weight [g/mol]: 394.60

Physical Properties

Property code	Value	Unit	Source
af	1.1175		Cheméo Relay (1.0)
hf	-4.86	kJ/mol	Cheméo Relay (1.0)
hvap	125.60	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-8.43		Cheméo Relay (1.0)
logp	8.638		Crippen Method
mcvol	351.210	ml/mol	McGowan Method
pc	1094.00	kPa	Cheméo Relay (1.0, beta)
tb	701.42	K	Cheméo Relay (1.0)
tc	961.25	K	Cheméo Relay (1.0)
tf	304.19	K	Cheméo Relay (1.0)
vc	1.296	m3/kmol	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37592895&Units=SI

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume