4-n-Pentanoyl-4-n'-heptadecanoyloxyazobenzene

Inchi: InChI=1S/C34H50N2O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-34(38)39-32-27-25
InchiKey: UXQRVZKVHTYICD-ULDVOPSXSA-N
Formula: C34H50N2O3
SMILES: CCCCCCCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CCCC)cc2)cc1
Mol. weight [g/mol]: 534.77
CAS: 120103-10-8

Physical Properties

Property code	Value	Unit	Source
hf	-605.13	kJ/mol	Joback Method
hvap	119.73	kJ/mol	Joback Method
log10ws	-12.02		Crippen Method
logp	11.252		Crippen Method
mcvol	467.070	ml/mol	McGowan Method
pc	624.06	kPa	Joback Method
tb	1320.00	K	Joback Method
tc	1663.41	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120103108&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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