

4-n-Pentanoyl-4-n'-undecanoyloxyazobenzene

Inchi: InChI=1S/C28H38N2O3/c1-3-5-7-8-9-10-11-12-14-28(32)33-26-21-19-25(20-22-26)30-29
InchiKey: VIDMLFVDTSEABM-QVIHXGFCSA-N
Formula: C28H38N2O3
SMILES: CCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CCCC)cc2)cc1
Mol. weight [g/mol]: 450.61
CAS: 120103-04-0

Physical Properties

Property code	Value	Unit	Source
hf	-481.29	kJ/mol	Joback Method
hvap	106.37	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.911		Crippen Method
mcvol	382.530	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
tb	1182.72	K	Joback Method
tc	1450.70	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.85	kJ/mol	359.00	NIST Webbook
sfust	63.66	J/molxK	359.00	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C120103040&Units=SI>

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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