4-n-Pentanoyl-4-n'-pentanoyloxyazobenzene

Inchi: InChI=1S/C22H26N2O3/c1-3-5-7-21(25)17-9-11-18(12-10-17)23-24-19-13-15-20(16-14-1
InchiKey: IFNWLIHOKYCDEY-WCWDXBQESA-N
Formula: C22H26N2O3
SMILES: CCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CCCC)cc2)cc1
Mol. weight [g/mol]: 366.45
CAS: 120102-98-9

Physical Properties

Property code	Value	Unit	Source
hf	-357.45	kJ/mol	Joback Method
hvap	93.01	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.571		Crippen Method
mcvol	297.990	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
tb	1045.44	K	Joback Method
tc	1288.62	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	7.10	kJ/mol	355.10	NIST Webbook
sfust	20.00	J/mol×K	355.10	NIST Webbook

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=C120102989&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature