4-n-Pentanoyl-4-n'-butanoyloxyazobenzene

Inchi: InChI=1S/C21H24N2O3/c1-3-5-7-20(24)16-8-10-17(11-9-16)22-23-18-12-14-19(15-13-18
InchiKey: IGGPWVPSOWNDOT-GHVJWSGMSA-N
Formula: C21H24N2O3
SMILES: CCCCC(=O)c1ccc(N=Nc2ccc(OC(=O)CCC)cc2)cc1
Mol. weight [g/mol]: 352.43
CAS: 120122-98-7

Physical Properties

Property code	Value	Unit	Source
hf	-336.81	kJ/mol	Joback Method
hvap	90.79	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.180		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
tb	1022.56	K	Joback Method
tc	1265.36	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.23	kJ/mol	373.30	NIST Webbook
sfust	38.12	J/mol×K	373.30	NIST Webbook

Sources

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=C120122987&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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