4-Propionyl-4'-n-heptadecanoyloxyazobenzene

Inchi: InChI=1S/C32H46N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-32(36)37-30-25-23-
InchiKey: VRFWDWVCSYKDIU-JEIPZWNWSA-N
Formula: C32H46N2O3
SMILES: CCCCCCCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 506.72
CAS: 76204-55-2

Physical Properties

Property code	Value	Unit	Source
hf	-563.85	kJ/mol	Joback Method
hvap	115.27	kJ/mol	Joback Method
log10ws	-11.18		Crippen Method
logp	10.471		Crippen Method
mcvol	438.890	ml/mol	McGowan Method
pc	688.53	kPa	Joback Method
tb	1274.24	K	Joback Method
tc	1585.57	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	58.74	kJ/mol	379.65	NIST Webbook
sfust	154.70	J/mol×K	379.65	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204552&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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