4-Propionyl-4'-n-hexadecanoyloxyazobenzene

Inchi: InChI=1S/C31H44N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-31(35)36-29-24-22-28(
InchiKey: ZEDTZWNGRUOMLX-ULIFNZDWSA-N
Formula: C31H44N2O3
SMILES: CCCCCCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 492.69
CAS: 76204-56-3

Physical Properties

Property code	Value	Unit	Source
hf	-543.21	kJ/mol	Joback Method
hvap	113.05	kJ/mol	Joback Method
log10ws	-10.77		Crippen Method
logp	10.081		Crippen Method
mcvol	424.800	ml/mol	McGowan Method
pc	724.57	kPa	Joback Method
tb	1251.36	K	Joback Method
tc	1549.43	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	53.01	kJ/mol	378.65	NIST Webbook
sfust	140.00	J/mol×K	378.65	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204563&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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