4-Propionyl-4'-n-pentadecanoyloxyazobenzene

Inchi: InChI=1S/C30H42N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-30(34)35-28-23-21-27(22-
InchiKey: LRMHNVQVSWAZPG-QNEJGDQOSA-N
Formula: C30H42N2O3
SMILES: CCCCCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 478.67
CAS: 76204-57-4

Physical Properties

Property code	Value	Unit	Source
hf	-522.57	kJ/mol	Joback Method
hvap	110.82	kJ/mol	Joback Method
log10ws	-10.35		Crippen Method
logp	9.691		Crippen Method
mcvol	410.710	ml/mol	McGowan Method
pc	763.52	kPa	Joback Method
tb	1228.48	K	Joback Method
tc	1514.97	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	51.51	kJ/mol	376.65	NIST Webbook
sfust	136.70	J/mol×K	376.65	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204574&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