4-Propionyl-4'-n-dodecanoyloxyazobenzene

Inchi: InChI=1S/C27H36N2O3/c1-3-5-6-7-8-9-10-11-12-13-27(31)32-25-20-18-24(19-21-25)29-
InchiKey: ONGYSCFQDCQYMA-ZQHSETAFSA-N
Formula: C27H36N2O3
SMILES: CCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 436.59
CAS: 76204-60-9

Physical Properties

Property code	Value	Unit	Source
hf	-460.65	kJ/mol	Joback Method
hvap	104.14	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	8.521		Crippen Method
mcvol	368.440	ml/mol	McGowan Method
pc	901.26	kPa	Joback Method
tb	1159.84	K	Joback Method
tc	1420.68	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	38.07	kJ/mol	373.65	NIST Webbook
sfust	101.90	J/mol×K	373.65	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204609&Units=SI

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