4-Propionyl-4'-n-undecanoyloxyazobenzene

Inchi: InChI=1S/C26H34N2O3/c1-3-5-6-7-8-9-10-11-12-26(30)31-24-19-17-23(18-20-24)28-27-
InchiKey: NBDZKMQIGUBQIA-BYYHNAKLSA-N
Formula: C26H34N2O3
SMILES: CCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 422.56
CAS: 76204-61-0

Physical Properties

Property code	Value	Unit	Source
hf	-440.01	kJ/mol	Joback Method
hvap	101.92	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.131		Crippen Method
mcvol	354.350	ml/mol	McGowan Method
pc	955.55	kPa	Joback Method
tb	1136.96	K	Joback Method
tc	1391.96	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	37.49	kJ/mol	370.65	NIST Webbook
sfust	101.10	J/mol×K	370.65	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=C76204610&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