

4-Propionyl-4'-n-tridecanoyloxyazobenzene

Inchi: InChI=1S/C28H38N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-28(32)33-26-21-19-25(20-22-26)
InchiKey: FFEMJSHTGJQOPX-QVIHXGFCSA-N
Formula: C28H38N2O3
SMILES: CCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 450.61
CAS: 76204-59-6

Physical Properties

Property code	Value	Unit	Source
hf	-481.29	kJ/mol	Joback Method
hvac	106.37	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.911		Crippen Method
mccvol	382.530	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
tb	1182.72	K	Joback Method
tc	1450.70	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	44.77	kJ/mol	374.65	NIST Webbook
sfust	119.50	J/molxK	374.65	NIST Webbook

Sources

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=C76204596&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvac:	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

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