

4-Propionyl-4'-n-octadecanoyloxyazobenzene

Inchi:	InChI=1S/C33H48N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-33(37)38-31-26
InchiKey:	PPCXODISASLTSK-XAHDOWKMSA-N
Formula:	C33H48N2O3
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]:	520.75
CAS:	76212-79-8

Physical Properties

Property code	Value	Unit	Source
hf	-584.49	kJ/mol	Joback Method
hvap	117.50	kJ/mol	Joback Method
log10ws	-11.60		Crippen Method
logp	10.862		Crippen Method
mcvol	452.980	ml/mol	McGowan Method
pc	655.11	kPa	Joback Method
tb	1297.12	K	Joback Method
tc	1623.52	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	59.62	kJ/mol	380.65	NIST Webbook
sfust	156.60	J/mol×K	380.65	NIST Webbook

Sources

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=C76212798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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