

4-Propionyl-4'-n-hexanoyloxyazobenzene

Inchi:	InChI=1S/C21H24N2O3/c1-3-5-6-7-21(25)26-19-14-12-18(13-15-19)23-22-17-10-8-16(9)
InchiKey:	WFBAYATFGFPGM-GHVJWSGMSA-N
Formula:	C21H24N2O3
SMILES:	CCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]:	352.43
CAS:	76204-66-5

Physical Properties

Property code	Value	Unit	Source
hf	-336.81	kJ/mol	Joback Method
hvap	90.79	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.180		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
tb	1022.56	K	Joback Method
tc	1265.36	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.79	kJ/mol	372.15	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C76204665&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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