

# 4-Propionyl-4'-n-heptanoyloxyazobenzene

Inchi:	InChI=1S/C22H26N2O3/c1-3-5-6-7-8-22(26)27-20-15-13-19(14-16-20)24-23-18-11-9-17
InchiKey:	MLESXCMZPBJKKZ-WCWDXBQESA-N
Formula:	C22H26N2O3
SMILES:	CCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]:	366.45
CAS:	76204-65-4

## Physical Properties

Property code	Value	Unit	Source
hf	-357.45	kJ/mol	Joback Method
hvap	93.01	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.571		Crippen Method
mcvol	297.990	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
tb	1045.44	K	Joback Method
tc	1288.62	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.81	kJ/mol	365.15	NIST Webbook
sfust	67.95	J/mol×K	365.15	NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204654&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307i>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

# Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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