

4-Propionyl-4'-n-butanoyloxyazobenzene

Inchi:	InChI=1S/C19H20N2O3/c1-3-5-19(23)24-17-12-10-16(11-13-17)21-20-15-8-6-14(7-9-15)
InchiKey:	HLEPKMLIJXPC-QZQOTICOSA-N
Formula:	C19H20N2O3
SMILES:	CCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]:	324.37
CAS:	76204-68-7

Physical Properties

Property code	Value	Unit	Source
hf	-295.53	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.400		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
tb	976.80	K	Joback Method
tc	1221.54	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	15.02	kJ/mol	366.00	NIST Webbook
sfust	41.04	J/molxK	366.00	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=C76204687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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