

# 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

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204654&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature       |
| <b>hvac:</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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