

# Flurazepam M (bisdesethyl)-H<sub>2</sub>O, hydrolysis, acetylated

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C19H18ClFN2O3/c1-12(24)22-9-10-23(13(2)25)18-8-7-14(20)11-16(18)19(26) |
| InchiKey:            | DWCBOQDXAIRNCQ-UHFFFAOYSA-N   |
| Formula:             | C19H18ClFN2O3   |
| SMILES:              | CC(=O)N(CCN=C(C)O)c1ccc(Cl)cc1C(=O)c1ccccc1F                                    |
| Mol. weight [g/mol]: | 376.81  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -446.12 | kJ/mol | Joback Method  |
| hvap          | 103.60  | kJ/mol | Joback Method  |
| log10ws       | -4.79   |        | Crippen Method |
| logp          | 4.039   |        | Crippen Method |
| mcvol         | 269.730 | ml/mol | McGowan Method |
| pc            | 1749.21 | kPa    | Joback Method  |
| rinpol        | 2460.00 |        | NIST Webbook   |
| rinpol        | 2460.00 |        | NIST Webbook   |
| tb            | 1028.04 | K      | Joback Method  |
| tc            | 1264.52 | K      | Joback Method  |

## Sources

|                 |   |
|-----------------|---|
| 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=R313050&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R313050&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|       |   |
|-------|---|
| hf:   | Enthalpy of formation at standard conditions    |
| hvap: | Enthalpy of vaporization at standard conditions |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mvol:</b>    | McGowan's characteristic volume     |
| <b>pc:</b>      | Critical Pressure                   |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |

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