

# Valdecoxib

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Bextra<br>4-(5-Methyl-3-phenyl-4-isoxazolyl)benzenesulfonamide (valdecoxib)     |
| <b>Inchi:</b>               | InChI=1S/C16H14N2O3S/c1-11-15(12-7-9-14(10-8-12)22(17,19)20)16(18-21-11)13-5-3- |
| <b>InchiKey:</b>            | LNPDTQAFDNKSHK-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H14N2O3S   |
| <b>SMILES:</b>              | <chem>Cc1onc(-c2ccccc2)c1-c1ccc(S(N)(=O)=O)cc1</chem>                           |
| <b>Mol. weight [g/mol]:</b> | 314.36  |
| <b>CAS:</b>                 | 181695-72-7   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -10.35  |        | Crippen Method |
| logp          | 2.964   |        | Crippen Method |
| mvol          | 223.240 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit   | Temperature [K] | Source       |
|---------------|-------|--------|-----------------|--------------|
| hfust         | 30.35 | kJ/mol | 446.40          | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C181695727&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C181695727&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                       |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |

# Legend

|                 |   |
|-----------------|---|
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l        |
| <b>logp:</b>    | Octanol/Water partition coefficient       |
| <b>mcvol:</b>   | McGowan's characteristic volume           |

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