

# Desethylatrazine

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1-methylethyl)-<br>2-Chloro-4-amino-6-(isopropylamino)-s-triazine<br>6-chloro-N-propan-2-yl-1,3,5-triazine-2,4-diamine<br>Atrazine M (des-ethyl)<br>Atrazine desethyl<br>Deethylatrazine<br>s-Triazine, 2-amino-4-chloro-6-(isopropylamino)- |
| <b>Inchi:</b>               | InChI=1S/C6H10ClN5/c1-3(2)9-6-11-4(7)10-5(8)12-6/h3H,1-2H3,(H3,8,9,10,11,12)   |
| <b>InchiKey:</b>            | DFWFIQKMSFGDCQ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C6H10ClN5  |
| <b>SMILES:</b>              | CC(C)Nc1nc(N)nc(Cl)n1  |
| <b>Mol. weight [g/mol]:</b> | 187.63   |
| <b>CAS:</b>                 | 6190-65-4  |

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| log10ws       | -1.77   |        | Aqueous Solubility Prediction Method |
| logp          | 0.927   |        | Crippen Method                       |
| mcvol         | 133.780 | ml/mol | McGowan Method                       |
| rinpol        | 1665.00 |        | NIST Webbook                         |
| rinpol        | 281.83  |        | NIST Webbook                         |
| rinpol        | 1665.00 |        | NIST Webbook                         |

## Sources

|  |   |
|--|---|
| <b>Crippen Method:</b>                       | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>   |
| <b>Aqueous Solubility Prediction Method:</b> | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a> |
| <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=C6190654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6190654&amp;Units=SI</a>   |

# Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <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>rinpol:</b>  | Non-polar retention indices         |

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