

# Bromacetamide, N-octadecyl-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C20H40BrNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-20(23)19-21 |
| <b>InchiKey:</b>            | DKNQDZVKKFNKSU-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C20H40BrNO   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCN=C(O)CBr  |
| <b>Mol. weight [g/mol]:</b> | 390.44   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -509.60 | kJ/mol | Joback Method  |
| hvap          | 86.62   | kJ/mol | Joback Method  |
| log10ws       | -7.61   |        | Crippen Method |
| logp          | 7.599   |        | Crippen Method |
| mcvol         | 321.710 | ml/mol | McGowan Method |
| pc            | 1056.20 | kPa    | Joback Method  |
| rinpol        | 2767.00 |        | NIST Webbook   |
| rinpol        | 2767.00 |        | NIST Webbook   |
| tb            | 891.90  | K      | Joback Method  |
| tc            | 1091.95 | K      | Joback Method  |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=U407084&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407084&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hf:</b>   | Enthalpy of formation at standard conditions    |
| <b>hvap:</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>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |

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