

# Pentanoic acid, 5-bromo-

|                      |                                                                                                                                                      |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 5-Bromovaleric acid<br>5-Bromopentanoic acid<br>2-Bromovaleric acid<br>5-Bromo-n-valeric acid<br>«delta»-Bromovaleric acid<br>Valeric acid, 5-bromo- |
| Inchi:               | InChI=1S/C5H9BrO2/c6-4-2-1-3-5(7)8/h1-4H2,(H,7,8)                                                                                                    |
| InchiKey:            | WNXNUPJZWYOKMW-UHFFFAOYSA-N                                                                                                                          |
| Formula:             | C5H9BrO2                                                                                                                                             |
| SMILES:              | O=C(O)CCCCBr                                                                                                                                         |
| Mol. weight [g/mol]: | 181.03                                                                                                                                               |
| CAS:                 | 2067-33-6                                                                                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -260.20 | kJ/mol  | Joback Method  |
| hf            | -385.01 | kJ/mol  | Joback Method  |
| hfus          | 19.68   | kJ/mol  | Joback Method  |
| hvap          | 56.58   | kJ/mol  | Joback Method  |
| log10ws       | -1.45   |         | Crippen Method |
| logp          | 1.636   |         | Crippen Method |
| mcvol         | 106.250 | ml/mol  | McGowan Method |
| pc            | 4602.62 | kPa     | Joback Method  |
| tb            | 526.01  | K       | Joback Method  |
| tc            | 713.17  | K       | Joback Method  |
| tf            | 316.66  | K       | Joback Method  |
| vc            | 0.403   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 214.72 | J/mol×K | 526.01          | Joback Method |
| cpg           | 248.15 | J/mol×K | 681.98          | Joback Method |
| cpg           | 242.15 | J/mol×K | 650.78          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 235.83    | J/mol×K | 619.59 | Joback Method |
| cpg   | 229.16    | J/mol×K | 588.40 | Joback Method |
| cpg   | 222.13    | J/mol×K | 557.20 | Joback Method |
| cpg   | 253.83    | J/mol×K | 713.17 | Joback Method |
| dvisc | 0.0002075 | Pa×s    | 526.01 | Joback Method |
| dvisc | 0.0003124 | Pa×s    | 491.12 | Joback Method |
| dvisc | 0.0005010 | Pa×s    | 456.23 | Joback Method |
| dvisc | 0.0008686 | Pa×s    | 421.33 | Joback Method |
| dvisc | 0.0016633 | Pa×s    | 386.44 | Joback Method |
| dvisc | 0.0036236 | Pa×s    | 351.55 | Joback Method |
| dvisc | 0.0093719 | Pa×s    | 316.66 | 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=C2067336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2067336&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>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion 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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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