

# Bromoacetyl chloride

|                      |                                    |
|----------------------|------------------------------------|
| Other names:         | Acetyl chloride, bromo-            |
| Inchi:               | InChI=1S/C2H2BrClO/c3-1-2(4)5/h1H2 |
| InchiKey:            | SYZRZLUNWVNNNV-UHFFFAOYSA-N        |
| Formula:             | C2H2BrClO                          |
| SMILES:              | O=C(Cl)CBr                         |
| Mol. weight [g/mol]: | 157.39                             |
| CAS:                 | 22118-09-8                         |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | -160.57       | kJ/mol  | Joback Method  |
| hf            | -186.60       | kJ/mol  | Joback Method  |
| hfus          | 12.02         | kJ/mol  | Joback Method  |
| hvap          | 37.61         | kJ/mol  | Joback Method  |
| log10ws       | -1.02         |         | Crippen Method |
| logp          | 1.147         |         | Crippen Method |
| mcvol         | 70.350        | ml/mol  | McGowan Method |
| pc            | 5782.94       | kPa     | Joback Method  |
| tb            | 400.20        | K       | NIST Webbook   |
| tb            | 400.00 ± 3.00 | K       | NIST Webbook   |
| tc            | 614.35        | K       | Joback Method  |
| tf            | 251.95        | K       | Joback Method  |
| vc            | 0.265         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 91.80  | J/mol×K | 402.62          | Joback Method |
| cpg           | 95.42  | J/mol×K | 437.91          | Joback Method |
| cpg           | 98.80  | J/mol×K | 473.20          | Joback Method |
| cpg           | 101.96 | J/mol×K | 508.48          | Joback Method |
| cpg           | 104.89 | J/mol×K | 543.77          | Joback Method |
| cpg           | 107.62 | J/mol×K | 579.06          | Joback Method |
| cpg           | 110.16 | J/mol×K | 614.35          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0030973 | Pa×s | 251.95 | Joback Method |
| dvisc | 0.0020107 | Pa×s | 277.06 | Joback Method |
| dvisc | 0.0014024 | Pa×s | 302.17 | Joback Method |
| dvisc | 0.0010338 | Pa×s | 327.28 | Joback Method |
| dvisc | 0.0007959 | Pa×s | 352.40 | Joback Method |
| dvisc | 0.0006345 | Pa×s | 377.51 | Joback Method |
| dvisc | 0.0005203 | Pa×s | 402.62 | 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=C22118098&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22118098&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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