# 4-Bromobutyric acid, 2,2,2-trichloroethyl ester

**Inchi:** InChI=1S/C6H8BrCl3O2/c7-3-1-2-5(11)12-4-6(8,9)10/h1-4H2
**InchiKey:** BMKUEJKAWLEGCS-UHFFFAOYSA-N
**Formula:** C6H8BrCl3O2
**SMILES:** O=C(CCCBr)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 298.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -252.91 | kJ/mol | Joback Method |
| hf | -441.61 | kJ/mol | Joback Method |
| hfus | 24.55 | kJ/mol | Joback Method |
| hvap | 56.40 | kJ/mol | Joback Method |
| log10ws | -3.19 | | Crippen Method |
| logp | 3.075 | | Crippen Method |
| mcvol | 157.060 | ml/mol | McGowan Method |
| pc | 3188.33 | kPa | Joback Method |
| rinpol | 1554.00 | | NIST Webbook |
| tb | 588.19 | K | Joback Method |
| tc | 809.68 | K | Joback Method |
| tf | 381.52 | K | Joback Method |
| vc | 0.594 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 306.20 | J/mol×K | 588.19 | Joback Method |
| cpg | 314.72 | J/mol×K | 625.11 | Joback Method |
| cpg | 322.60 | J/mol×K | 662.02 | Joback Method |
| cpg | 329.88 | J/mol×K | 698.94 | Joback Method |
| cpg | 336.59 | J/mol×K | 735.85 | Joback Method |
| cpg | 342.79 | J/mol×K | 772.77 | Joback Method |
| cpg | 348.50 | J/mol×K | 809.68 | Joback Method |
| dvisc | 0.0019798 | Pa×s | 381.52 | Joback Method |
| dvisc | 0.0012062 | Pa×s | 415.96 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0007928 | Pa×s | 450.41 | Joback Method |
| dvisc | 0.0005531 | Pa×s | 484.86 | Joback Method |
| dvisc | 0.0004047 | Pa×s | 519.30 | Joback Method |
| dvisc | 0.0003079 | Pa×s | 553.75 | Joback Method |
| dvisc | 0.0002418 | Pa×s | 588.19 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354687&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |