# Acetic acid, bromo-, 2-methylpropyl ester

| | |
|---|---|
| **Other names:** | Bromoacetic acid, 2-methylpropyl ester |
| | Isobutyl bromoacetate |
| **Inchi:** | InChI=1S/C6H11BrO2/c1-5(2)4-9-6(8)3-7/h5H,3-4H2,1-2H3 |
| **InchiKey:** | UOUQDZFAJUNYQQ-UHFFFAOYSA-N |
| **Formula:** | C6H11BrO2 |
| **SMILES:** | CC(C)COC(=O)CBr |
| **Mol. weight [g/mol]:** | 195.05 |
| **CAS:** | 59956-48-8 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -222.40 | kJ/mol | Joback Method |
| hf | -390.92 | kJ/mol | Joback Method |
| hfus | 15.85 | kJ/mol | Joback Method |
| hvap | 44.15 | kJ/mol | Joback Method |
| log10ws | -1.39 | | Crippen Method |
| logp | 1.580 | | Crippen Method |
| mcvol | 120.340 | ml/mol | McGowan Method |
| pc | 3581.35 | kPa | Joback Method |
| rinpol | 1025.80 | | NIST Webbook |
| rinpol | 1021.00 | | NIST Webbook |
| rinpol | 1021.00 | | NIST Webbook |
| rinpol | 1021.00 | | NIST Webbook |
| rinpol | 1021.00 | | NIST Webbook |
| rinpol | 1025.80 | | NIST Webbook |
| ripol | 1488.00 | | NIST Webbook |
| ripol | 1488.00 | | NIST Webbook |
| tb | 478.69 | K | Joback Method |
| tc | 677.47 | K | Joback Method |
| tf | 274.34 | K | Joback Method |
| vc | 0.452 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 235.52 | J/mol×K | 478.69 | Joback Method |
| cpg | 245.58 | J/mol×K | 511.82 | Joback Method |
| cpg | 255.20 | J/mol×K | 544.95 | Joback Method |
| cpg | 264.38 | J/mol×K | 578.08 | Joback Method |
| cpg | 273.13 | J/mol×K | 611.21 | Joback Method |
| cpg | 281.46 | J/mol×K | 644.34 | Joback Method |
| cpg | 289.37 | J/mol×K | 677.47 | Joback Method |
| dvisc | 0.0035442 | Pa×s | 274.34 | Joback Method |
| dvisc | 0.0018866 | Pa×s | 308.40 | Joback Method |
| dvisc | 0.0011385 | Pa×s | 342.46 | Joback Method |
| dvisc | 0.0007528 | Pa×s | 376.51 | Joback Method |
| dvisc | 0.0005331 | Pa×s | 410.57 | Joback Method |
| dvisc | 0.0003980 | Pa×s | 444.63 | Joback Method |
| dvisc | 0.0003098 | Pa×s | 478.69 | Joback Method |

# Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C59956488&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**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
**ripol:** Polar retention indices

| | |
|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |