# Bromoacetic acid, dodecyl ester

**Other names:** Dodecyl bromoacetate
**Inchi:** InChI=1S/C14H27BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-14(16)13-15/h2-13H2,1H3
**InchiKey:** QIPFGFYXERNTNP-UHFFFAOYSA-N
**Formula:** C14H27BrO2
**SMILES:** CCCCCCCCCCCCOC(=O)CBr
**Mol. weight [g/mol]:** 307.27
**CAS:** 3674-07-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -152.60 | kJ/mol | Joback Method |
| hf | -550.76 | kJ/mol | Joback Method |
| hfus | 40.09 | kJ/mol | Joback Method |
| hvap | 62.35 | kJ/mol | Joback Method |
| log10ws | -4.98 | | Crippen Method |
| logp | 4.845 | | Crippen Method |
| mcvol | 233.060 | ml/mol | McGowan Method |
| pc | 1670.06 | kPa | Joback Method |
| rinpol | 1885.30 | | NIST Webbook |
| rinpol | 1885.30 | | NIST Webbook |
| tb | 662.17 | K | Joback Method |
| tc | 841.70 | K | Joback Method |
| tf | 379.50 | K | Joback Method |
| vc | 0.905 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 617.88 | J/mol×K | 662.17 | Joback Method |
| cpg | 633.84 | J/mol×K | 692.09 | Joback Method |
| cpg | 649.05 | J/mol×K | 722.01 | Joback Method |
| cpg | 663.54 | J/mol×K | 751.94 | Joback Method |
| cpg | 677.31 | J/mol×K | 781.86 | Joback Method |
| cpg | 690.40 | J/mol×K | 811.78 | Joback Method |

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|---|---|---|---|---|
| cpg | 702.81 | J/mol×K | 841.70 | Joback Method |
| dvisc | 0.0017594 | Pa×s | 379.50 | Joback Method |
| dvisc | 0.0009057 | Pa×s | 426.61 | Joback Method |
| dvisc | 0.0005321 | Pa×s | 473.72 | Joback Method |
| dvisc | 0.0003442 | Pa×s | 520.84 | Joback Method |
| dvisc | 0.0002393 | Pa×s | 567.95 | Joback Method |
| dvisc | 0.0001759 | Pa×s | 615.06 | Joback Method |
| dvisc | 0.0001351 | Pa×s | 662.17 | Joback Method |

# Sources

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|---|---|
| **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=C3674075&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |

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