# Glutaric acid, monochloride, 4-bromophenyl ester

**Inchi:** InChI=1S/C11H10BrClO3/c12-8-4-6-9(7-5-8)16-11(15)3-1-2-10(13)14/h4-7H,1-3H2
**InchiKey:** AOWDQVYPNSNHTI-UHFFFAOYSA-N
**Formula:** C11H10BrClO3
**SMILES:** O=C(Cl)CCCC(=O)Oc1ccc(Br)cc1
**Mol. weight [g/mol]:** 305.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -215.93 | kJ/mol | Joback Method |
| hf | -392.10 | kJ/mol | Joback Method |
| hfus | 31.77 | kJ/mol | Joback Method |
| hvap | 69.74 | kJ/mol | Joback Method |
| log10ws | -4.13 | | Crippen Method |
| logp | 3.290 | | Crippen Method |
| mcvol | 180.840 | ml/mol | McGowan Method |
| pc | 3028.94 | kPa | Joback Method |
| rinpol | 2051.00 | | NIST Webbook |
| rinpol | 2051.00 | | NIST Webbook |
| tb | 716.49 | K | Joback Method |
| tc | 948.49 | K | Joback Method |
| tf | 464.48 | K | Joback Method |
| vc | 0.684 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.49 | J/mol×K | 716.49 | Joback Method |
| cpg | 430.07 | J/mol×K | 755.16 | Joback Method |
| cpg | 439.82 | J/mol×K | 793.82 | Joback Method |
| cpg | 448.78 | J/mol×K | 832.49 | Joback Method |
| cpg | 456.97 | J/mol×K | 871.16 | Joback Method |
| cpg | 464.43 | J/mol×K | 909.82 | Joback Method |
| cpg | 471.18 | J/mol×K | 948.49 | Joback Method |
| dvisc | 0.0010764 | Pa×s | 464.48 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0007014 | Pa×s | 506.48 | Joback Method |
| dvisc | 0.0004880 | Pa×s | 548.48 | Joback Method |
| dvisc | 0.0003576 | Pa×s | 590.49 | Joback Method |
| dvisc | 0.0002730 | Pa×s | 632.49 | Joback Method |
| dvisc | 0.0002156 | Pa×s | 674.49 | Joback Method |
| dvisc | 0.0001750 | Pa×s | 716.49 | 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=U358735&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 |