# Glutaric acid, cyclohexylmethyl 4-bromophenyl ester

**Inchi:** InChI=1S/C18H23BrO4/c19-15-9-11-16(12-10-15)23-18(21)8-4-7-17(20)22-13-14-5-2-1-3

**InchiKey:** AYQGJYGOZMWWGO-UHFFFAOYSA-N

**Formula:** C18H23BrO4

**SMILES:** O=C(CCCC(=O)Oc1ccc(Br)cc1)OCC1CCCCC1

**Mol. weight [g/mol]:** 383.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -225.61 | kJ/mol | Joback Method |
| hf | -598.74 | kJ/mol | Joback Method |
| hfus | 38.72 | kJ/mol | Joback Method |
| hvap | 83.78 | kJ/mol | Joback Method |
| log10ws | -5.65 | | Crippen Method |
| logp | 4.648 | | Crippen Method |
| mcvol | 262.240 | ml/mol | McGowan Method |
| pc | 1950.95 | kPa | Joback Method |
| rinpol | 2723.00 | | NIST Webbook |
| rinpol | 2723.00 | | NIST Webbook |
| tb | 881.19 | K | Joback Method |
| tc | 1113.91 | K | Joback Method |
| tf | 543.06 | K | Joback Method |
| vc | 0.979 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 794.88 | J/mol×K | 881.19 | Joback Method |
| cpg | 809.65 | J/mol×K | 919.98 | Joback Method |
| cpg | 822.97 | J/mol×K | 958.76 | Joback Method |
| cpg | 834.88 | J/mol×K | 997.55 | Joback Method |
| cpg | 845.42 | J/mol×K | 1036.34 | Joback Method |
| cpg | 854.64 | J/mol×K | 1075.12 | Joback Method |
| cpg | 862.57 | J/mol×K | 1113.91 | Joback Method |
| dvisc | 0.0005460 | Pa×s | 543.06 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003174 | Pa×s | 599.41 | Joback Method |
| dvisc | 0.0002026 | Pa×s | 655.77 | Joback Method |
| dvisc | 0.0001388 | Pa×s | 712.12 | Joback Method |
| dvisc | 0.0001005 | Pa×s | 768.48 | Joback Method |
| dvisc | 0.0000761 | Pa×s | 824.83 | Joback Method |
| dvisc | 0.0000597 | Pa×s | 881.19 | 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=U393294&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |