# Glutaric acid, di(4-bromo-2-methoxyphenyl) ester

**Inchi:** InChI=1S/C19H18Br2O6/c1-24-16-10-12(20)6-8-14(16)26-18(22)4-3-5-19(23)27-15-9-7-1
**InchiKey:** YHCNGQMRBCAIFD-UHFFFAOYSA-N
**Formula:** C19H18Br2O6
**SMILES:** COc1cc(Br)ccc1OC(=O)CCCC(=O)Oc1ccc(Br)cc1OC
**Mol. weight [g/mol]:** 502.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -353.80 | kJ/mol | Joback Method |
| hf | -709.69 | kJ/mol | Joback Method |
| hfus | 50.01 | kJ/mol | Joback Method |
| hvap | 101.09 | kJ/mol | Joback Method |
| log10ws | -6.73 | | Crippen Method |
| logp | 4.910 | | Crippen Method |
| mcvol | 292.670 | ml/mol | McGowan Method |
| pc | 1985.89 | kPa | Joback Method |
| rinpol | 3319.00 | | NIST Webbook |
| rinpol | 3319.00 | | NIST Webbook |
| tb | 1037.14 | K | Joback Method |
| tc | 1283.28 | K | Joback Method |
| tf | 715.19 | K | Joback Method |
| vc | 1.091 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 828.84 | J/mol×K | 1037.14 | Joback Method |
| cpg | 851.16 | J/mol×K | 1242.26 | Joback Method |
| cpg | 849.90 | J/mol×K | 1201.23 | Joback Method |
| cpg | 847.03 | J/mol×K | 1160.21 | Joback Method |
| cpg | 842.56 | J/mol×K | 1119.19 | Joback Method |
| cpg | 836.50 | J/mol×K | 1078.16 | Joback Method |
| cpg | 850.83 | J/mol×K | 1283.28 | Joback Method |
| dvisc | 0.0000227 | Pa×s | 1037.14 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000273 | Pa×s | 983.48 | Joback Method |
| dvisc | 0.0000336 | Pa×s | 929.82 | Joback Method |
| dvisc | 0.0000423 | Pa×s | 876.17 | Joback Method |
| dvisc | 0.0000550 | Pa×s | 822.51 | Joback Method |
| dvisc | 0.0000741 | Pa×s | 768.85 | Joback Method |
| dvisc | 0.0001043 | Pa×s | 715.19 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393897&Units=SI |

# 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 |