# Glutaric acid, 2-(3-bromophenyl)ethyl tridecyl ester

**Inchi:** InChI=1S/C26H41BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-20-30-25(28)17-14-18-26(29)31-21-

**InchiKey:** KKWSEAANAXJWNV-UHFFFAOYSA-N

**Formula:** C26H41BrO4

**SMILES:** CCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1cccc(Br)c1

**Mol. weight [g/mol]:** 497.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -182.70 | kJ/mol | Joback Method |
| hf | -818.18 | kJ/mol | Joback Method |
| hfus | 67.61 | kJ/mol | Joback Method |
| hvap | 101.15 | kJ/mol | Joback Method |
| log10ws | -8.70 | | Crippen Method |
| logp | 7.559 | | Crippen Method |
| mcvol | 385.820 | ml/mol | McGowan Method |
| pc | 954.37 | kPa | Joback Method |
| rinpol | 3441.00 | | NIST Webbook |
| rinpol | 3441.00 | | NIST Webbook |
| tb | 1044.68 | K | Joback Method |
| tc | 1281.15 | K | Joback Method |
| tf | 625.84 | K | Joback Method |
| vc | 1.494 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1283.30 | J/mol×K | 1044.68 | Joback Method |
| cpg | 1348.36 | J/mol×K | 1241.74 | Joback Method |
| cpg | 1338.15 | J/mol×K | 1202.33 | Joback Method |
| cpg | 1326.62 | J/mol×K | 1162.92 | Joback Method |
| cpg | 1313.68 | J/mol×K | 1123.50 | Joback Method |
| cpg | 1299.27 | J/mol×K | 1084.09 | Joback Method |
| cpg | 1357.32 | J/mol×K | 1281.15 | Joback Method |
| dvisc | 0.0000169 | Pa×s | 1044.68 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000219 | Pa×s | 974.87 | Joback Method |
| dvisc | 0.0000295 | Pa×s | 905.07 | Joback Method |
| dvisc | 0.0000417 | Pa×s | 835.26 | Joback Method |
| dvisc | 0.0000629 | Pa×s | 765.45 | Joback Method |
| dvisc | 0.0001030 | Pa×s | 695.65 | Joback Method |
| dvisc | 0.0001884 | Pa×s | 625.84 | 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=U377216&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 |