# Glutaric acid, 3-bromobenzyl isobutyl ester

**Inchi:** InChI=1S/C16H21BrO4/c1-12(2)10-20-15(18)7-4-8-16(19)21-11-13-5-3-6-14(17)9-13/h3,
**InchiKey:** GJKCACKRGKRXOY-UHFFFAOYSA-N
**Formula:** C16H21BrO4
**SMILES:** CC(C)COC(=O)CCCC(=O)OCc1cccc(Br)c1
**Mol. weight [g/mol]:** 357.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -269.34 | kJ/mol | Joback Method |
| hf | -617.06 | kJ/mol | Joback Method |
| hfus | 38.18 | kJ/mol | Joback Method |
| hvap | 78.51 | kJ/mol | Joback Method |
| log10ws | -4.76 | | Crippen Method |
| logp | 3.862 | | Crippen Method |
| mcvol | 244.920 | ml/mol | McGowan Method |
| pc | 1942.37 | kPa | Joback Method |
| rinpol | 2578.00 | | NIST Webbook |
| rinpol | 2578.00 | | NIST Webbook |
| tb | 815.44 | K | Joback Method |
| tc | 1030.25 | K | Joback Method |
| tf | 498.14 | K | Joback Method |
| vc | 0.927 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.18 | J/mol×K | 815.44 | Joback Method |
| cpg | 746.45 | J/mol×K | 994.45 | Joback Method |
| cpg | 736.79 | J/mol×K | 958.65 | Joback Method |
| cpg | 726.16 | J/mol×K | 922.85 | Joback Method |
| cpg | 714.53 | J/mol×K | 887.04 | Joback Method |
| cpg | 701.88 | J/mol×K | 851.24 | Joback Method |
| cpg | 755.17 | J/mol×K | 1030.25 | Joback Method |
| dvisc | 0.0000706 | Pa×s | 815.44 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000900 | Pa×s | 762.56 | Joback Method |
| dvisc | 0.0001191 | Pa×s | 709.67 | Joback Method |
| dvisc | 0.0001647 | Pa×s | 656.79 | Joback Method |
| dvisc | 0.0002410 | Pa×s | 603.91 | Joback Method |
| dvisc | 0.0003796 | Pa×s | 551.02 | Joback Method |
| dvisc | 0.0006585 | Pa×s | 498.14 | 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=U377678&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 |