# Glutaric acid, 2-bromo-5-fluorobenzyl propyl ester

**Inchi:** InChI=1S/C15H18BrFO4/c1-2-8-20-14(18)4-3-5-15(19)21-10-11-9-12(17)6-7-13(11)16/h
**InchiKey:** LVPUBKGDESYPGY-UHFFFAOYSA-N
**Formula:** C15H18BrFO4
**SMILES:** CCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
**Mol. weight [g/mol]:** 361.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -479.76 | kJ/mol | Joback Method |
| hf | -798.72 | kJ/mol | Joback Method |
| hfus | 41.81 | kJ/mol | Joback Method |
| hvap | 76.51 | kJ/mol | Joback Method |
| log10ws | -4.92 | | Crippen Method |
| logp | 3.755 | | Crippen Method |
| mcvol | 232.600 | ml/mol | McGowan Method |
| pc | 1991.21 | kPa | Joback Method |
| rinpol | 2211.00 | | NIST Webbook |
| rinpol | 2211.00 | | NIST Webbook |
| tb | 797.25 | K | Joback Method |
| tc | 1005.05 | K | Joback Method |
| tf | 514.98 | K | Joback Method |
| vc | 0.895 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 638.56 | J/mol×K | 797.25 | Joback Method |
| cpg | 651.18 | J/mol×K | 831.88 | Joback Method |
| cpg | 662.90 | J/mol×K | 866.52 | Joback Method |
| cpg | 673.72 | J/mol×K | 901.15 | Joback Method |
| cpg | 683.65 | J/mol×K | 935.78 | Joback Method |
| cpg | 692.71 | J/mol×K | 970.42 | Joback Method |
| cpg | 700.91 | J/mol×K | 1005.05 | Joback Method |

# Sources

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|---|---|
| **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=U377059&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |