# Glutaric acid, 4-bromophenyl 1,1,1-trifluoroprop-2-yl ester

**Inchi:** InChI=1S/C14H14BrF3O4/c1-9(14(16,17)18)21-12(19)3-2-4-13(20)22-11-7-5-10(15)6-8-1

**InchiKey:** AZPNFEBOVLFPRR-UHFFFAOYSA-N

**Formula:** C14H14BrF3O4

**SMILES:** CC(OC(=O)CCCC(=O)Oc1ccc(Br)cc1)C(F)(F)F

**Mol. weight [g/mol]:** 383.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -867.77 | kJ/mol | Joback Method |
| hf | -1172.86 | kJ/mol | Joback Method |
| hfus | 34.83 | kJ/mol | Joback Method |
| hvap | 70.31 | kJ/mol | Joback Method |
| log10ws | -5.10 | | Crippen Method |
| logp | 4.019 | | Crippen Method |
| mcvol | 222.050 | ml/mol | McGowan Method |
| pc | 2079.33 | kPa | Joback Method |
| rinpol | 1973.00 | | NIST Webbook |
| rinpol | 1973.00 | | NIST Webbook |
| tb | 764.26 | K | Joback Method |
| tc | 970.41 | K | Joback Method |
| tf | 479.79 | K | Joback Method |
| vc | 0.859 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 603.78 | J/mol×K | 764.26 | Joback Method |
| cpg | 615.48 | J/mol×K | 798.62 | Joback Method |
| cpg | 626.30 | J/mol×K | 832.98 | Joback Method |
| cpg | 636.25 | J/mol×K | 867.33 | Joback Method |
| cpg | 645.40 | J/mol×K | 901.69 | Joback Method |
| cpg | 653.76 | J/mol×K | 936.05 | Joback Method |
| cpg | 661.37 | J/mol×K | 970.41 | 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=U393282&Units=SI |

# 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 |