

# Glutaric acid, hex-4-yn-3-yl 4-bromophenyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C17H19BrO4/c1-3-6-14(4-2)21-16(19)7-5-8-17(20)22-15-11-9-13(18)10-12-15 |
| InchiKey:            | XDBCSDVGZSIQAW-UHFFFAOYSA-N  |
| Formula:             | C17H19BrO4   |
| SMILES:              | CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(Br)cc1   |
| Mol. weight [g/mol]: | 367.23   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -58.12  | kJ/mol               | Joback Method  |
| hf            | -365.40 | kJ/mol               | Joback Method  |
| hfus          | 43.90   | kJ/mol               | Joback Method  |
| hvap          | 82.89   | kJ/mol               | Joback Method  |
| log10ws       | -5.48   |                      | Crippen Method |
| logp          | 3.870   |                      | Crippen Method |
| mvol          | 250.410 | ml/mol               | McGowan Method |
| pc            | 2056.76 | kPa                  | Joback Method  |
| rinpol        | 2441.00 |                      | NIST Webbook   |
| rinpol        | 2441.00 |                      | NIST Webbook   |
| tb            | 847.32  | K                    | Joback Method  |
| tc            | 1077.29 | K                    | Joback Method  |
| tf            | 615.51  | K                    | Joback Method  |
| vc            | 0.946   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 692.19 | J/mol×K | 847.32          | Joback Method |
| cpg           | 705.44 | J/mol×K | 885.65          | Joback Method |
| cpg           | 717.55 | J/mol×K | 923.98          | Joback Method |
| cpg           | 728.56 | J/mol×K | 962.30          | Joback Method |
| cpg           | 738.49 | J/mol×K | 1000.63         | Joback Method |
| cpg           | 747.37 | J/mol×K | 1038.96         | Joback Method |
| cpg           | 755.22 | J/mol×K | 1077.29         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393290&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393290&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvp:</b>     | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinp:</b>    | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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