# Succinic acid, 5-bromo-2-methoxybenzyl propyl ester

**Inchi:** InChI=1S/C15H19BrO5/c1-3-8-20-14(17)6-7-15(18)21-10-11-9-12(16)4-5-13(11)19-2/h4-

**InchiKey:** UGHHRHZFBRUFSA-UHFFFAOYSA-N

**Formula:** C15H19BrO5

**SMILES:** CCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC

**Mol. weight [g/mol]:** 359.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -389.95 | kJ/mol | Joback Method |
| hf | -734.83 | kJ/mol | Joback Method |
| hfus | 39.92 | kJ/mol | Joback Method |
| hvap | 79.74 | kJ/mol | Joback Method |
| log10ws | -4.29 | | Crippen Method |
| logp | 3.234 | | Crippen Method |
| mcvol | 236.700 | ml/mol | McGowan Method |
| pc | 2041.91 | kPa | Joback Method |
| rinpol | 2357.00 | | NIST Webbook |
| rinpol | 2357.00 | | NIST Webbook |
| tb | 820.40 | K | Joback Method |
| tc | 1033.88 | K | Joback Method |
| tf | 536.62 | K | Joback Method |
| vc | 0.895 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 657.39 | J/mol×K | 820.40 | Joback Method |
| cpg | 670.12 | J/mol×K | 855.98 | Joback Method |
| cpg | 681.83 | J/mol×K | 891.56 | Joback Method |
| cpg | 692.52 | J/mol×K | 927.14 | Joback Method |
| cpg | 702.18 | J/mol×K | 962.72 | Joback Method |
| cpg | 710.81 | J/mol×K | 998.30 | Joback Method |
| cpg | 718.41 | J/mol×K | 1033.88 | Joback Method |
| dvisc | 0.0004079 | Pa×s | 536.62 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002674 | Pa×s | 583.92 | Joback Method |
| dvisc | 0.0001868 | Pa×s | 631.21 | Joback Method |
| dvisc | 0.0001371 | Pa×s | 678.51 | Joback Method |
| dvisc | 0.0001048 | Pa×s | 725.81 | Joback Method |
| dvisc | 0.0000828 | Pa×s | 773.10 | Joback Method |
| dvisc | 0.0000672 | Pa×s | 820.40 | 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=U381070&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 |