# Succinic acid, 2,2-dichloroethyl 4-bromo-2-methoxyphenyl ester

**Inchi:** InChI=1S/C13H13BrCl2O5/c1-19-10-6-8(14)2-3-9(10)21-13(18)5-4-12(17)20-7-11(15)16/

**InchiKey:** AYZQEKNFFHVXEF-UHFFFAOYSA-N

**Formula:** C13H13BrCl2O5

**SMILES:** COc1cc(Br)ccc1OC(=O)CCC(=O)OCC(Cl)Cl

**Mol. weight [g/mol]:** 400.05

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -433.09 | kJ/mol | Joback Method |
| hf | -730.31 | kJ/mol | Joback Method |
| hfus | 39.61 | kJ/mol | Joback Method |
| hvap | 83.67 | kJ/mol | Joback Method |
| log10ws | -4.52 | | Crippen Method |
| logp | 3.490 | | Crippen Method |
| mcvol | 233.000 | ml/mol | McGowan Method |
| pc | 2295.91 | kPa | Joback Method |
| rinpol | 2551.00 | | NIST Webbook |
| rinpol | 2551.00 | | NIST Webbook |
| tb | 849.06 | K | Joback Method |
| tc | 1076.28 | K | Joback Method |
| tf | 558.92 | K | Joback Method |
| vc | 0.875 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 591.72 | J/mol×K | 849.06 | Joback Method |
| cpg | 601.62 | J/mol×K | 886.93 | Joback Method |
| cpg | 610.51 | J/mol×K | 924.80 | Joback Method |
| cpg | 618.36 | J/mol×K | 962.67 | Joback Method |
| cpg | 625.18 | J/mol×K | 1000.54 | Joback Method |
| cpg | 630.97 | J/mol×K | 1038.41 | Joback Method |
| cpg | 635.72 | J/mol×K | 1076.28 | Joback Method |
| dvisc | 0.0003763 | Pa×s | 558.92 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002458 | Pa×s | 607.28 | Joback Method |
| dvisc | 0.0001710 | Pa×s | 655.63 | Joback Method |
| dvisc | 0.0001250 | Pa×s | 703.99 | Joback Method |
| dvisc | 0.0000951 | Pa×s | 752.35 | Joback Method |
| dvisc | 0.0000748 | Pa×s | 800.70 | Joback Method |
| dvisc | 0.0000605 | Pa×s | 849.06 | Joback Method |

# Sources

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|---|---|
| **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=U390915&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 |