# Malonic acid, 2-butyl isobutyl ester

**Inchi:** InChI=1S/C11H20O4/c1-5-9(4)15-11(13)6-10(12)14-7-8(2)3/h8-9H,5-7H2,1-4H3
**InchiKey:** LNZJNFXUORACEO-UHFFFAOYSA-N
**Formula:** C11H20O4
**SMILES:** CCC(C)OC(=O)CC(=O)OCC(C)C
**Mol. weight [g/mol]:** 216.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -430.98 | kJ/mol | Joback Method |
| hf | -770.53 | kJ/mol | Joback Method |
| hfus | 22.77 | kJ/mol | Joback Method |
| hvap | 57.62 | kJ/mol | Joback Method |
| log10ws | -2.02 | | Crippen Method |
| logp | 1.917 | | Crippen Method |
| mcvol | 180.730 | ml/mol | McGowan Method |
| pc | 2131.49 | kPa | Joback Method |
| rinpol | 1298.00 | | NIST Webbook |
| rinpol | 1298.00 | | NIST Webbook |
| tb | 602.78 | K | Joback Method |
| tc | 787.66 | K | Joback Method |
| tf | 328.05 | K | Joback Method |
| vc | 0.688 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 465.83 | J/mol×K | 602.78 | Joback Method |
| cpg | 480.33 | J/mol×K | 633.59 | Joback Method |
| cpg | 494.18 | J/mol×K | 664.41 | Joback Method |
| cpg | 507.38 | J/mol×K | 695.22 | Joback Method |
| cpg | 519.94 | J/mol×K | 726.03 | Joback Method |
| cpg | 531.86 | J/mol×K | 756.85 | Joback Method |
| cpg | 543.12 | J/mol×K | 787.66 | Joback Method |
| dvisc | 0.0029767 | Pa×s | 328.05 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0013297 | Pa×s | 373.84 | Joback Method |
| dvisc | 0.0007082 | Pa×s | 419.63 | Joback Method |
| dvisc | 0.0004269 | Pa×s | 465.41 | Joback Method |
| dvisc | 0.0002818 | Pa×s | 511.20 | Joback Method |
| dvisc | 0.0001992 | Pa×s | 556.99 | Joback Method |
| dvisc | 0.0001484 | Pa×s | 602.78 | 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=U349068&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |

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