# Butanedioic acid, bis(2-methylpropyl) ester

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|---|---|
| **Other names:** | Succinic acid, diisobutyl ester |
| | Diisobutyl succinate |
| | Butanedioic acid, di-(2-methylpropyl) ester |
| | Diisobutyl butanedioate |
| **Inchi:** | InChI=1S/C12H22O4/c1-9(2)7-15-11(13)5-6-12(14)16-8-10(3)4/h9-10H,5-8H2,1-4H3 |
| **InchiKey:** | QCOAPBRVQHMEPF-UHFFFAOYSA-N |
| **Formula:** | C12H22O4 |
| **SMILES:** | CC(C)COC(=O)CCC(=O)OCC(C)C |
| **Mol. weight [g/mol]:** | 230.30 |
| **CAS:** | 925-06-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -422.56 | kJ/mol | Joback Method |
| hf | -791.17 | kJ/mol | Joback Method |
| hfus | 25.36 | kJ/mol | Joback Method |
| hvap | 59.84 | kJ/mol | Joback Method |
| log10ws | -2.09 | | Crippen Method |
| logp | 2.165 | | Crippen Method |
| mcvol | 194.820 | ml/mol | McGowan Method |
| pc | 1954.41 | kPa | Joback Method |
| rinpol | 1451.00 | | NIST Webbook |
| rinpol | 1447.00 | | NIST Webbook |
| rinpol | 1452.00 | | NIST Webbook |
| rinpol | 1447.00 | | NIST Webbook |
| rinpol | 1451.00 | | NIST Webbook |
| rinpol | 1450.00 | | NIST Webbook |
| tb | 625.66 | K | Joback Method |
| tc | 808.87 | K | Joback Method |
| tf | 339.32 | K | Joback Method |
| vc | 0.744 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 516.81 | J/mol×K | 625.66 | Joback Method |
| cpg | 585.47 | J/mol×K | 778.33 | Joback Method |
| cpg | 573.11 | J/mol×K | 747.80 | Joback Method |
| cpg | 560.07 | J/mol×K | 717.26 | Joback Method |
| cpg | 546.34 | J/mol×K | 686.73 | Joback Method |
| cpg | 531.92 | J/mol×K | 656.19 | Joback Method |
| cpg | 597.13 | J/mol×K | 808.87 | Joback Method |
| dvisc | 0.0001321 | Pa×s | 625.66 | Joback Method |
| dvisc | 0.0001778 | Pa×s | 577.94 | Joback Method |
| dvisc | 0.0002525 | Pa×s | 530.21 | Joback Method |
| dvisc | 0.0003843 | Pa×s | 482.49 | Joback Method |
| dvisc | 0.0006416 | Pa×s | 434.77 | Joback Method |
| dvisc | 0.0012154 | Pa×s | 387.04 | Joback Method |
| dvisc | 0.0027555 | Pa×s | 339.32 | Joback Method |

# Sources

**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=C925064&Units=SI

# 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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