# 2-methylbutyl 2-methylbutanoate-d-3

**Inchi:** InChI=1S/C10H20O2/c1-5-8(3)7-12-10(11)9(4)6-2/h8-9H,5-7H2,1-4H3/i2D3
**InchiKey:** PVYFCGRBIREQLL-BMSJAHLVSA-N
**Formula:** C10H17D3O2
**SMILES:** CCC(C)COC(=O)C(C)CC
**Mol. weight [g/mol]:** 175.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -205.48 | kJ/mol | Joback Method |
| hf | -505.09 | kJ/mol | Joback Method |
| hfus | 17.40 | kJ/mol | Joback Method |
| hvap | 46.23 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 2.622 | | Crippen Method |
| mcvol | 159.200 | ml/mol | McGowan Method |
| pc | 2233.41 | kPa | Joback Method |
| ripol | 1283.00 | | NIST Webbook |
| ripol | 1283.00 | | NIST Webbook |
| tb | 503.61 | K | Joback Method |
| tc | 682.96 | K | Joback Method |
| tf | 244.62 | K | Joback Method |
| vc | 0.608 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 368.51 | J/mol×K | 503.61 | Joback Method |
| cpg | 383.39 | J/mol×K | 533.50 | Joback Method |
| cpg | 397.67 | J/mol×K | 563.39 | Joback Method |
| cpg | 411.38 | J/mol×K | 593.28 | Joback Method |
| cpg | 424.51 | J/mol×K | 623.18 | Joback Method |
| cpg | 437.08 | J/mol×K | 653.07 | Joback Method |
| cpg | 449.08 | J/mol×K | 682.96 | Joback Method |
| dvisc | 0.0070487 | Pa×s | 244.62 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0024917 | Pa×s | 287.79 | Joback Method |
| dvisc | 0.0011553 | Pa×s | 330.95 | Joback Method |
| dvisc | 0.0006396 | Pa×s | 374.12 | Joback Method |
| dvisc | 0.0004002 | Pa×s | 417.28 | Joback Method |
| dvisc | 0.0002734 | Pa×s | 460.44 | Joback Method |
| dvisc | 0.0001994 | Pa×s | 503.61 | 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=R322539&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |