# 2-Hexenoic acid, butyl ester, (E)-

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|---|---|
| **Other names:** | Butyl (2E)-2-hexenoate |
| | Butyl (E)-2-hexenoate |
| | Butyl trans-hex-2-enoate |
| **Inchi:** | InChI=1S/C10H18O2/c1-3-5-7-8-10(11)12-9-6-4-2/h7-8H,3-6,9H2,1-2H3/b8-7+ |
| **InchiKey:** | OPVSKLFHWQRZKR-BQYQJAHWSA-N |
| **Formula:** | C10H18O2 |
| **SMILES:** | CCCC=CC(=O)OCCCC |
| **Mol. weight [g/mol]:** | 170.25 |
| **CAS:** | 54411-16-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -120.38 | kJ/mol | Joback Method |
| hf | -377.31 | kJ/mol | Joback Method |
| hfus | 24.64 | kJ/mol | Joback Method |
| hvap | 46.97 | kJ/mol | Joback Method |
| log10ws | -2.72 | | Crippen Method |
| logp | 2.686 | | Crippen Method |
| mcvol | 154.900 | ml/mol | McGowan Method |
| pc | 2311.39 | kPa | Joback Method |
| rinpol | 1243.00 | | NIST Webbook |
| rinpol | 1243.00 | | NIST Webbook |
| tb | 508.65 | K | Joback Method |
| tc | 688.43 | K | Joback Method |
| tf | 269.54 | K | Joback Method |
| vc | 0.600 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 350.74 | J/mol×K | 508.65 | Joback Method |
| cpg | 364.56 | J/mol×K | 538.61 | Joback Method |
| cpg | 377.79 | J/mol×K | 568.58 | Joback Method |
| cpg | 390.44 | J/mol×K | 598.54 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 402.54 | J/mol×K | 628.50 | Joback Method |
| cpg | 414.10 | J/mol×K | 658.47 | Joback Method |
| cpg | 425.13 | J/mol×K | 688.43 | Joback Method |
| dvisc | 0.0030444 | Pa×s | 269.54 | Joback Method |
| dvisc | 0.0014196 | Pa×s | 309.39 | Joback Method |
| dvisc | 0.0007878 | Pa×s | 349.24 | Joback Method |
| dvisc | 0.0004933 | Pa×s | 389.10 | Joback Method |
| dvisc | 0.0003369 | Pa×s | 428.95 | Joback Method |
| dvisc | 0.0002455 | Pa×s | 468.80 | Joback Method |
| dvisc | 0.0001880 | Pa×s | 508.65 | Joback Method |

# Sources

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|---|---|
| **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=C54411164&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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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