

# 4-Methylhexyl isobutyrate

|                      |                                                                     |
|----------------------|---------------------------------------------------------------------|
| Inchi:               | InChI=1S/C11H22O2/c1-5-10(4)7-6-8-13-11(12)9(2)3/h9-10H,5-8H2,1-4H3 |
| InchiKey:            | XSGWKQYSBYNOGB-UHFFFAOYSA-N                                         |
| Formula:             | C11H22O2                                                            |
| SMILES:              | CCC(C)CCCOC(=O)C(C)C                                                |
| Mol. weight [g/mol]: | 186.29                                                              |
| CAS:                 | 1215127-77-7                                                        |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -197.06 | kJ/mol  | Joback Method  |
| hf            | -525.73 | kJ/mol  | Joback Method  |
| hfus          | 19.99   | kJ/mol  | Joback Method  |
| hvap          | 48.46   | kJ/mol  | Joback Method  |
| log10ws       | -2.81   |         | Crippen Method |
| logp          | 3.012   |         | Crippen Method |
| mcvol         | 173.290 | ml/mol  | McGowan Method |
| pc            | 2043.76 | kPa     | Joback Method  |
| rinpol        | 1220.00 |         | NIST Webbook   |
| rinpol        | 1220.00 |         | NIST Webbook   |
| tb            | 526.49  | K       | Joback Method  |
| tc            | 704.16  | K       | Joback Method  |
| tf            | 255.89  | K       | Joback Method  |
| vc            | 0.663   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 415.72 | J/mol×K | 526.49          | Joback Method |
| cpg           | 487.83 | J/mol×K | 674.54          | Joback Method |
| cpg           | 474.64 | J/mol×K | 644.93          | Joback Method |
| cpg           | 460.84 | J/mol×K | 615.32          | Joback Method |
| cpg           | 446.42 | J/mol×K | 585.71          | Joback Method |
| cpg           | 431.38 | J/mol×K | 556.10          | Joback Method |
| cpg           | 500.43 | J/mol×K | 704.16          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001825 | Pa×s | 526.49 | Joback Method |
| dvisc | 0.0002510 | Pa×s | 481.39 | Joback Method |
| dvisc | 0.0003687 | Pa×s | 436.29 | Joback Method |
| dvisc | 0.0005917 | Pa×s | 391.19 | Joback Method |
| dvisc | 0.0010741 | Pa×s | 346.09 | Joback Method |
| dvisc | 0.0023315 | Pa×s | 300.99 | Joback Method |
| dvisc | 0.0066509 | Pa×s | 255.89 | Joback Method |

## Sources

|                        |                                                                                                                                                 |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C121512777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C121512777&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                       |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                           |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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