

Undecanoic acid, 2-methyl-, methyl ester

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| Other names: | Methyl ester of 2-methylundecanoic acid Methyl 2-methylundecanoate |
| Inchi: | InChI=1S/C13H26O2/c1-4-5-6-7-8-9-10-11-12(2)13(14)15-3/h12H,4-11H2,1-3H3 |
| InchiKey: | KGVPRVBZKYLXFP-UHFFFAOYSA-N |
| Formula: | C13H26O2 |
| SMILES: | CCCCCCCCC(C)C(=O)OC |
| Mol. weight [g/mol]: | 214.34 |
| CAS: | 55955-69-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -177.78 | kJ/mol | Joback Method |
| hf | -561.73 | kJ/mol | Joback Method |
| hfus | 28.69 | kJ/mol | Joback Method |
| hvap | 53.30 | kJ/mol | Joback Method |
| log10ws | -3.88 | | Crippen Method |
| logp | 3.936 | | Crippen Method |
| mcvol | 201.470 | ml/mol | McGowan Method |
| pc | 1718.88 | kPa | Joback Method |
| ripol | 2629.00 | | NIST Webbook |
| ripol | 2629.00 | | NIST Webbook |
| tb | 572.69 | K | Joback Method |
| tc | 744.36 | K | Joback Method |
| tf | 293.43 | K | Joback Method |
| vc | 0.781 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 515.10 | J/molxK | 572.69 | Joback Method |
| cpg | 531.74 | J/molxK | 601.30 | Joback Method |
| cpg | 547.70 | J/molxK | 629.91 | Joback Method |
| cpg | 563.00 | J/molxK | 658.53 | Joback Method |
| cpg | 577.64 | J/molxK | 687.14 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 591.64 | J/molxK | 715.75 | Joback Method |
| cpg | 605.00 | J/molxK | 744.36 | Joback Method |
| dvisc | 0.0040106 | Paxs | 293.43 | Joback Method |
| dvisc | 0.0016218 | Paxs | 339.97 | Joback Method |
| dvisc | 0.0008156 | Paxs | 386.52 | Joback Method |
| dvisc | 0.0004755 | Paxs | 433.06 | Joback Method |
| dvisc | 0.0003078 | Paxs | 479.60 | Joback Method |
| dvisc | 0.0002152 | Paxs | 526.15 | Joback Method |
| dvisc | 0.0001594 | Paxs | 572.69 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C55955696&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/34-337-0/Undecanoic-acid-2-methyl-methyl-ester.pdf>

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