# 2-Ethylbutyric acid, 2-methylpentyl ester

**Inchi:** InChI=1S/C12H24O2/c1-5-8-10(4)9-14-12(13)11(6-2)7-3/h10-11H,5-9H2,1-4H3
**InchiKey:** CMLILCIKJQYHFF-UHFFFAOYSA-N
**Formula:** C12H24O2
**SMILES:** CCCC(C)COC(=O)C(CC)CC
**Mol. weight [g/mol]:** 200.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -188.64 | kJ/mol | Joback Method |
| hf | -546.37 | kJ/mol | Joback Method |
| hfus | 22.58 | kJ/mol | Joback Method |
| hvap | 50.69 | kJ/mol | Joback Method |
| log10ws | -3.22 | | Crippen Method |
| logp | 3.402 | | Crippen Method |
| mcvol | 187.380 | ml/mol | McGowan Method |
| pc | 1877.28 | kPa | Joback Method |
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1182.00 | | NIST Webbook |
| tb | 549.37 | K | Joback Method |
| tc | 725.46 | K | Joback Method |
| tf | 267.16 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 464.71 | J/mol×K | 549.37 | Joback Method |
| cpg | 539.94 | J/mol×K | 696.11 | Joback Method |
| cpg | 526.20 | J/mol×K | 666.76 | Joback Method |
| cpg | 511.82 | J/mol×K | 637.42 | Joback Method |
| cpg | 496.78 | J/mol×K | 608.07 | Joback Method |
| cpg | 481.08 | J/mol×K | 578.72 | Joback Method |
| cpg | 553.06 | J/mol×K | 725.46 | Joback Method |
| dvisc | 0.0001657 | Pa×s | 549.37 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002285 | Pa×s | 502.33 | Joback Method |
| dvisc | 0.0003366 | Pa×s | 455.30 | Joback Method |
| dvisc | 0.0005423 | Pa×s | 408.26 | Joback Method |
| dvisc | 0.0009890 | Pa×s | 361.23 | Joback Method |
| dvisc | 0.0021594 | Pa×s | 314.19 | Joback Method |
| dvisc | 0.0062070 | Pa×s | 267.16 | 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=U369773&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