

ethyl dotriacontanoate

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|-----------------------------|--|
| Inchi: | InChI=1S/C34H68O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25 |
| InchiKey: | IWELHCMIKMQCSY-UHFFFAOYSA-N |
| Formula: | C34H68O2 |
| SMILES: | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCC |
| Mol. weight [g/mol]: | 508.90 |
| CAS: | 29030-82-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 1.48 | kJ/mol | Joback Method |
| hf | -989.89 | kJ/mol | Joback Method |
| hfus | 86.60 | kJ/mol | Joback Method |
| hvap | 100.43 | kJ/mol | Joback Method |
| log10ws | -12.92 | | Crippen Method |
| logp | 12.272 | | Crippen Method |
| mcvol | 497.360 | ml/mol | McGowan Method |
| pc | 508.18 | kPa | Joback Method |
| rinpol | 3582.84 | | NIST Webbook |
| rinpol | 3582.84 | | NIST Webbook |
| tb | 1053.61 | K | Joback Method |
| tc | 1347.22 | K | Joback Method |
| tf | 545.10 | K | Joback Method |
| vc | 1.964 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1818.58 | J/mol×K | 1053.61 | Joback Method |
| cpg | 1947.21 | J/mol×K | 1298.29 | Joback Method |
| cpg | 1926.37 | J/mol×K | 1249.35 | Joback Method |
| cpg | 1903.31 | J/mol×K | 1200.42 | Joback Method |
| cpg | 1877.82 | J/mol×K | 1151.48 | Joback Method |
| cpg | 1849.65 | J/mol×K | 1102.55 | Joback Method |
| cpg | 1966.09 | J/mol×K | 1347.22 | Joback Method |

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|-------|-----------|------|---------|---------------|
| dvisc | 0.0000089 | Paxs | 1053.61 | Joback Method |
| dvisc | 0.0000123 | Paxs | 968.86 | Joback Method |
| dvisc | 0.0000180 | Paxs | 884.11 | Joback Method |
| dvisc | 0.0000287 | Paxs | 799.36 | Joback Method |
| dvisc | 0.0000510 | Paxs | 714.60 | Joback Method |
| dvisc | 0.0001060 | Paxs | 629.85 | Joback Method |
| dvisc | 0.0002762 | Paxs | 545.10 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C29030828&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| mvol: | 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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