

9-Octadecenoic acid, 12-hydroxy-, methyl ester, [R-(Z)]-

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| Other names: | 12-Hydroxy-9-octadecenoic acid methyl ester 9-octadecenoic acid, 12-hydroxy-, [R]-, methyl ester Flexricin P-1 Methyl ricinolate Ricinoleic acid methyl ester [R]-methyl 12-hydroxy-9-octadecenoate methyl ricinoleate |
| Inchi: | InChI=1S/C19H36O3/c1-3-4-5-12-15-18(20)16-13-10-8-6-7-9-11-14-17-19(21)22-2/h10,1 |
| InchiKey: | XKGDWZQXVZSXAO-GFBZKKKVSA-N |
| Formula: | C19H36O3 |
| SMILES: | CCCCCCC(O)CC=CCCCCCCCC(=O)OC |
| Mol. weight [g/mol]: | 312.49 |
| CAS: | 141-24-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|---|
| cpl | 696.53 | J/molxK | Energies of combustion and standard molar enthalpies of formation of ricinoleic acid and methyl ricinoleate |
| gf | -183.86 | kJ/mol | Joback Method |
| hf | -720.58 | kJ/mol | Joback Method |
| hfus | 48.52 | kJ/mol | Joback Method |
| hvap | 83.29 | kJ/mol | Joback Method |
| log10ws | -5.87 | | Crippen Method |
| logp | 5.168 | | Crippen Method |
| mcvol | 287.580 | ml/mol | McGowan Method |
| pc | 1236.35 | kPa | Joback Method |
| tb | 806.31 | K | Joback Method |
| tc | 988.85 | K | Joback Method |
| tf | 416.79 | K | Joback Method |
| vc | 1.117 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|--|
| cpg | 964.47 | J/molxK | 928.00 | Joback Method |
| cpg | 934.70 | J/molxK | 867.16 | Joback Method |
| cpg | 918.57 | J/molxK | 836.73 | Joback Method |
| cpg | 901.55 | J/molxK | 806.31 | Joback Method |
| cpg | 978.17 | J/molxK | 958.43 | Joback Method |
| cpg | 991.13 | J/molxK | 988.85 | Joback Method |
| cpg | 949.99 | J/molxK | 897.58 | Joback Method |
| dvisc | 0.0003895 | Paxs | 481.71 | Joback Method |
| dvisc | 0.0001383 | Paxs | 546.63 | Joback Method |
| dvisc | 0.0000611 | Paxs | 611.55 | Joback Method |
| dvisc | 0.0000316 | Paxs | 676.47 | Joback Method |
| dvisc | 0.0000184 | Paxs | 741.39 | Joback Method |
| dvisc | 0.0000116 | Paxs | 806.31 | Joback Method |
| dvisc | 0.0015155 | Paxs | 416.79 | Joback Method |
| hvapt | 89.30 | kJ/mol | 498.00 | NIST Webbook |
| rho1 | 857.50 | kg/m3 | 383.23 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rho1 | 865.80 | kg/m3 | 373.26 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rho1 | 875.00 | kg/m3 | 363.38 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rho1 | 883.30 | kg/m3 | 353.06 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |

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|------|--------|-------|--------|--|
| rhoI | 895.80 | kg/m3 | 343.32 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rhoI | 904.00 | kg/m3 | 333.25 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rhoI | 910.30 | kg/m3 | 323.05 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rhoI | 916.70 | kg/m3 | 313.33 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rhoI | 921.20 | kg/m3 | 303.17 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |
| rhoI | 928.50 | kg/m3 | 293.16 | Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate |

Sources

Measurements and Correlations of the Density, Viscosity, and Vapor Pressure for Methyl Ricinoleate:

<https://www.doi.org/10.1021/acs.jced.5b00545>

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C141242&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Energies of combustion and standard molar enthalpies of formation of ricinoleic acid and methyl ricinoleate:

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1016/j.jct.2012.02.006>

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| cpl: | Liquid phase 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 |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rho: | Liquid Density |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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