# Tridecyl trifluoroacetate

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| **Other names:** | Tridecyl trifluoroacetate |
| | Tridecyl 2,2,2-trifluoroacetate |
| | 1-Tridecanol, trifluoroacetate |
| | Trifluoroacetic acid, tridecyl ester |
| **Inchi:** | InChI=1S/C15H27F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-14(19)15(16,17)18/h2-13H2, |
| **InchiKey:** | DKWJQENYIDPCEX-UHFFFAOYSA-N |
| **Formula:** | C15H27F3O2 |
| **SMILES:** | CCCCCCCCCCCCCOC(=O)C(F)(F)F |
| **Mol. weight [g/mol]:** | 296.37 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.7728 | | Cheméo Relay (1.0) |
| hf | -1247.17 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 39.22 | kJ/mol | Joback Method |
| hvap | 77.24 | kJ/mol | Cheméo Relay (1.0) |
| ie | 10.46 | eV | Cheméo Relay (1.0) |
| log10ws | -5.61 | | Cheméo Relay (1.0) |
| logp | 5.403 | | Crippen Method |
| mcvol | 234.960 | ml/mol | McGowan Method |
| pc | 1343.73 | kPa | Joback Method |
| rinpol | 1527.50 | | NIST Webbook |
| rinpol | 1525.00 | | NIST Webbook |
| tb | 518.20 | K | Cheméo Relay (1.0) |
| tc | 642.74 | K | Cheméo Relay (1.0) |
| tf | 269.02 | K | Cheméo Relay (1.0) |
| vc | 0.904 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 647.26 | J/mol×K | 613.47 | Joback Method |
| cpg | 663.52 | J/mol×K | 639.79 | Joback Method |
| cpg | 679.08 | J/mol×K | 666.12 | Joback Method |

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|---|---|---|---|---|
| cpg | 693.94 | J/mol×K | 692.44 | Joback Method |
| cpg | 708.13 | J/mol×K | 718.76 | Joback Method |
| cpg | 721.67 | J/mol×K | 745.09 | Joback Method |
| cpg | 734.58 | J/mol×K | 771.41 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C53800025&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |