# Pentadecafluorooctanoic acid, tridec-2-yn-1-yl ester

**Inchi:** InChI=1S/C21H23F15O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-38-14(37)15(22,23)16(24,25)1

**InchiKey:** GVXWEJCIBRQRKO-UHFFFAOYSA-N

**Formula:** C21H23F15O2

**SMILES:** CCCCCCCCCCC#CCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 592.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2807.45 | kJ/mol | Joback Method |
| hf | -3452.17 | kJ/mol | Joback Method |
| hfus | 50.36 | kJ/mol | Joback Method |
| hvap | 52.32 | kJ/mol | Joback Method |
| log10ws | -9.82 | | Crippen Method |
| logp | 8.438 | | Crippen Method |
| mcvol | 332.140 | ml/mol | McGowan Method |
| pc | 784.63 | kPa | Joback Method |
| rinpol | 1738.00 | | NIST Webbook |
| tb | 731.61 | K | Joback Method |
| tc | 895.75 | K | Joback Method |
| tf | 530.48 | K | Joback Method |
| vc | 1.391 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1048.93 | J/mol×K | 731.61 | Joback Method |
| cpg | 1064.10 | J/mol×K | 758.97 | Joback Method |
| cpg | 1078.29 | J/mol×K | 786.32 | Joback Method |
| cpg | 1091.58 | J/mol×K | 813.68 | Joback Method |
| cpg | 1104.07 | J/mol×K | 841.04 | Joback Method |
| cpg | 1115.85 | J/mol×K | 868.40 | Joback Method |
| cpg | 1127.01 | J/mol×K | 895.75 | Joback Method |

# Sources

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|---|---|
| **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=U406814&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |