# L-Cysteine, N,S-di(trifluoroacetyl)-, 2,2,3,3,3-pentafluoropropyl ester

**Inchi:** InChI=1S/C10H6F11NO4S/c11-7(12,10(19,20)21)2-26-4(23)3(22-5(24)8(13,14)15)1-27-6

**InchiKey:** DCQLIBWHNMOBAW-UHFFFAOYSA-N

**Formula:** C10H6F11NO4S

**SMILES:** O=C(OCC(F)(F)C(F)(F)F)C(CSC(=O)C(F)(F)F)NC(=O)C(F)(F)F

**Mol. weight [g/mol]:** 445.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2469.92 | kJ/mol | Joback Method |
| hf | -2821.84 | kJ/mol | Joback Method |
| hfus | 37.57 | kJ/mol | Joback Method |
| hvap | 59.20 | kJ/mol | Joback Method |
| log10ws | -3.91 | | Crippen Method |
| logp | 2.596 | | Crippen Method |
| mcvol | 208.140 | ml/mol | McGowan Method |
| pc | 1755.07 | kPa | Joback Method |
| rinpol | 1140.50 | | NIST Webbook |
| rinpol | 1140.50 | | NIST Webbook |
| tb | 709.79 | K | Joback Method |
| tc | 881.38 | K | Joback Method |
| tf | 462.71 | K | Joback Method |
| vc | 0.869 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 610.30 | J/mol×K | 709.79 | Joback Method |
| cpg | 618.70 | J/mol×K | 738.39 | Joback Method |
| cpg | 626.38 | J/mol×K | 766.99 | Joback Method |
| cpg | 633.40 | J/mol×K | 795.59 | Joback Method |
| cpg | 639.79 | J/mol×K | 824.18 | Joback Method |
| cpg | 645.61 | J/mol×K | 852.78 | Joback Method |
| cpg | 650.92 | J/mol×K | 881.38 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U352347&Units=SI |
| **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 |

# 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 |

Latest version available from:
https://www.chemeo.com/cid/40-293-2/L-Cysteine-N-S-di-trifluoroacetyl-2-2-3-3-3-pentafluoropropyl-ester.pdf
Generated by Cheméo on 2024-05-01 01:49:23.716554735 +0000 UTC m=+16817412.637132046.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.