# 2,4,5-T Isopropyl ester

**Other names:** Acetic acid, (2,4,5-trichlorophenoxy)-, 1-methylethyl ester
Acetic acid, (2,4,5-trichlorophenoxy)-, isopropyl ester
Isopropyl (2,4,5-trichlorophenoxy)acetate
Acetic acid, (2,4,5-trichlorophenoxy)-, 1-methyl ester
Acetic acid,(2,4,5-trichloropheoxy)-, isopropyl ester
**Inchi:** InChI=1S/C11H11Cl3O3/c1-6(2)17-11(15)5-16-10-4-8(13)7(12)3-9(10)14/h3-4,6H,5H2,1-
**InchiKey:** SXHQLHGHMREHMX-UHFFFAOYSA-N
**Formula:** C11H11Cl3O3
**SMILES:** CC(C)OC(=O)COc1cc(Cl)c(Cl)cc1Cl
**Mol. weight [g/mol]:** 297.56
**CAS:** 93-78-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -251.89 | kJ/mol | Joback Method |
| hf | -497.77 | kJ/mol | Joback Method |
| hfus | 30.16 | kJ/mol | Joback Method |
| hvap | 68.67 | kJ/mol | Joback Method |
| log10ws | -4.30 | | Crippen Method |
| logp | 3.977 | | Crippen Method |
| mcvol | 192.120 | ml/mol | McGowan Method |
| pc | 2351.92 | kPa | Joback Method |
| rinpol | 1825.00 | | NIST Webbook |
| rinpol | 1825.00 | | NIST Webbook |
| tb | 703.26 | K | Joback Method |
| tc | 927.66 | K | Joback Method |
| tf | 446.86 | K | Joback Method |
| vc | 0.727 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 443.25 | J/mol×K | 703.26 | Joback Method |
| cpg | 454.46 | J/mol×K | 740.66 | Joback Method |

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|---|---|---|---|---|
| cpg | 464.90 | J/mol×K | 778.06 | Joback Method |
| cpg | 474.56 | J/mol×K | 815.46 | Joback Method |
| cpg | 483.43 | J/mol×K | 852.86 | Joback Method |
| cpg | 491.50 | J/mol×K | 890.26 | Joback Method |
| cpg | 498.78 | J/mol×K | 927.66 | Joback Method |
| dvisc | 0.0007459 | Pa×s | 446.86 | Joback Method |
| dvisc | 0.0004789 | Pa×s | 489.59 | Joback Method |
| dvisc | 0.0003302 | Pa×s | 532.33 | Joback Method |
| dvisc | 0.0002406 | Pa×s | 575.06 | Joback Method |
| dvisc | 0.0001831 | Pa×s | 617.79 | Joback Method |
| dvisc | 0.0001444 | Pa×s | 660.53 | Joback Method |
| dvisc | 0.0001172 | Pa×s | 703.26 | Joback Method |

# Sources

| | |
|---|---|
| **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=C93787&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **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 |