# Butyl 2-(2,4,5-trichlorophenoxy)propionate

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|---|---|
| **Other names:** | n-Butyl ester of alpha-(2,4,5-trichlorophenoxy)propionic acid |
| | 2,4,5-TP, butyl ester |
| | Fenoprop, butyl ester |
| | butyl 2-(2,4,5-trichlorophenoxy)propionate |
| **Inchi:** | InChI=1S/C13H15Cl3O3/c1-3-4-5-18-13(17)8(2)19-12-7-10(15)9(14)6-11(12)16/h6-8H,3- |
| **InchiKey:** | VPXVRVAKKVBOLA-UHFFFAOYSA-N |
| **Formula:** | C13H15Cl3O3 |
| **SMILES:** | CCCCOC(=O)C(C)Oc1cc(Cl)c(Cl)cc1Cl |
| **Mol. weight [g/mol]:** | 325.62 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -611.00 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 35.34 | kJ/mol | Joback Method |
| hvap | 87.96 | kJ/mol | Cheméo Relay (1.0) |
| log10ws | -4.98 | | Cheméo Relay (1.0) |
| logp | 4.757 | | Crippen Method |
| mcvol | 220.300 | ml/mol | McGowan Method |
| pc | 1968.30 | kPa | Joback Method |
| rinpol | 2035.00 | | NIST Webbook |
| rinpol | 2035.00 | | NIST Webbook |
| tb | 577.02 | K | Cheméo Relay (1.0) |
| tf | 328.51 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 546.32 | J/mol×K | 749.02 | Joback Method |
| cpg | 607.15 | J/mol×K | 966.49 | Joback Method |
| cpg | 599.19 | J/mol×K | 930.25 | Joback Method |
| cpg | 590.36 | J/mol×K | 894.00 | Joback Method |
| cpg | 580.66 | J/mol×K | 857.76 | Joback Method |
| cpg | 570.08 | J/mol×K | 821.51 | Joback Method |
| cpg | 558.64 | J/mol×K | 785.27 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001931 | Pa×s | 609.21 | Joback Method |
| dvisc | 0.0000910 | Pa×s | 749.02 | Joback Method |
| dvisc | 0.0001131 | Pa×s | 702.42 | Joback Method |
| dvisc | 0.0001450 | Pa×s | 655.81 | Joback Method |
| dvisc | 0.0006417 | Pa×s | 469.40 | Joback Method |
| dvisc | 0.0002697 | Pa×s | 562.61 | Joback Method |
| dvisc | 0.0004000 | Pa×s | 516.00 | Joback Method |

# Sources

| | |
|---|---|
| **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):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13557987&Units=SI |
| **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 |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **tf:** | Normal melting (fusion) point |