# Acifluorfen, undecyl ester

**Inchi:** InChI=1S/C25H29ClF3NO5/c1-2-3-4-5-6-7-8-9-10-15-34-24(31)20-17-19(12-13-22(20)30
**InchiKey:** QCBMFQQJCBVDDB-UHFFFAOYSA-N
**Formula:** C25H29ClF3NO5
**SMILES:** CCCCCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 515.95

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -550.97 | kJ/mol | Joback Method |
| hf | -1132.75 | kJ/mol | Joback Method |
| hfus | 68.39 | kJ/mol | Joback Method |
| hvap | 107.24 | kJ/mol | Joback Method |
| log10ws | -9.97 | | Crippen Method |
| logp | 8.747 | | Crippen Method |
| mcvol | 363.870 | ml/mol | McGowan Method |
| pc | 1022.04 | kPa | Joback Method |
| rinpol | 3517.00 | | NIST Webbook |
| tb | 1127.24 | K | Joback Method |
| tc | 1380.83 | K | Joback Method |
| tf | 746.54 | K | Joback Method |
| vc | 1.435 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1204.67 | J/mol×K | 1127.24 | Joback Method |
| cpg | 1215.41 | J/mol×K | 1169.51 | Joback Method |
| cpg | 1224.79 | J/mol×K | 1211.77 | Joback Method |
| cpg | 1232.92 | J/mol×K | 1254.04 | Joback Method |
| cpg | 1239.90 | J/mol×K | 1296.30 | Joback Method |
| cpg | 1245.86 | J/mol×K | 1338.57 | Joback Method |
| cpg | 1250.88 | J/mol×K | 1380.83 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415150&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 |