# (E)-10-Dodecenoic acid, 9,12-dioxo, methyl ester, bis-PFB-oxime, # 1

**Inchi:** InChI=1S/C27H24F10N2O4/c1-41-17(40)10-6-4-2-3-5-8-14(39-43-13-16-20(30)24(34)27

**InchiKey:** ZGSYEMOJGIYNMK-HUXKIHLDSA-N

**Formula:** C27H24F10N2O4

**SMILES:** COC(=O)CCCCCCCC(C=CC=NOCc1c(F)c(F)c(F)c(F)c1F)=NOCc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 630.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -2440.72 | kJ/mol | Joback Method |
| hvap | 99.34 | kJ/mol | Joback Method |
| log10ws | -10.84 | | Crippen Method |
| logp | 7.613 | | Crippen Method |
| mcvol | 387.710 | ml/mol | McGowan Method |
| pc | 661.19 | kPa | Joback Method |
| rinpol | 3080.00 | | NIST Webbook |
| rinpol | 3080.00 | | NIST Webbook |
| tb | 1191.55 | K | Joback Method |
| tc | 1515.01 | K | Joback Method |

## Sources

**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=R554904&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

**hf:** Enthalpy of formation 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 |