

8E,10E-Dodecadien-1-yl acetate, adduct with 4-methyl-1,2,4-triazolin-3,5-dione

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|----------------------|---|
| Other names: | 7E,9Z-Dodecadienyl acetate + MTAD adduct |
| Inchi: | InChI=1S/C17H27N3O4/c1-4-14-10-11-15(9-7-5-6-8-12-24-13(2)21)20-17(23)18(3)16(22) |
| InchiKey: | KUESRSOKACDQIV-UHFFFAOYSA-N |
| Formula: | C17H27N3O4 |
| SMILES: | CCC1C=CC(CCCCCOC(C)=O)n2c(=O)n(C)c(=O)n21 |
| Mol. weight [g/mol]: | 337.41 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.85 | | Crippen Method |
| logp | 1.924 | | Crippen Method |
| mcvol | 264.890 | ml/mol | McGowan Method |
| rinpola | 2530.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U293260&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpola: | Non-polar retention indices |

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