9Z,11E-Tetradecadien-1-yl acetate, adduct with 4-methyl-1,2,4-triazolin-3,5-dione

Other names: 8-(8-Ethyl-2-methyl-1,3-dioxo-2,3,5,8-tetrahydro-1H-[1,2,4]triazolo[1,2-a]pyridazin-5-yl)oc
9Z,11E-Tetradecadienyl acetate + MTAD adduct
acetate, trans

Inchi: InChI=1S/C19H31N3O4/c1-4-16-12-13-17(22-19(25)20(3)18(24)21(16)22)11-9-7-5-6-8-1

InchiKey: AXICEVNXCZPIJY-UHFFFAOYSA-N

Formula: C19H31N3O4

SMILES: CCC1C=CC(CCCCCCCCOC(C)=O)n2c(=O)n(C)c(=O)n21

Mol. weight [g/mol]: 365.47

CAS: 131916-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	2.704		Crippen Method
mcvol	293.070	ml/mol	McGowan Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C131916262&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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