

Trichlopyr-2-butoxyethyl ester (TBE)

Inchi: InChI=1S/C13H16Cl3NO4/c1-2-3-4-19-5-6-20-11(18)8-21-13-10(15)7-9(14)12(16)17-13/
InchiKey: IVDRCZNVHVGQBHZ-UHFFFAOYSA-N
Formula: C13H16Cl3NO4
SMILES: CCCCOCCOC(=O)COc1nc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 356.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	3.780		Crippen Method
mcvol	236.150	ml/mol	McGowan Method
rinpola	2234.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R276416&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/60-751-1/Trichlopyr-2-butoxyethyl-ester-TBE.pdf>

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