1-chloroacetyl-2,3-dihydro-7-ethylindole

Inchi: InChI=1S/C10H10ClNO/c11-7-10(13)12-6-5-8-3-1-2-4-9(8)12/h1-4H,5-7H2
InchiKey: ARHQTTKUMFDVJJ-UHFFFAOYSA-N
Formula: C10H10ClNO
SMILES: O=C(CCl)N1CCc2ccccc21
Mol. weight [g/mol]: 195.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	1.815		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R408509&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.