

O-Methyl-O-(2-chloro-1,1-difluoroethyl)ethanethio

Inchi: InChI=1S/C5H10ClF2O2PS/c1-3-11(12,9-2)10-5(7,8)4-6/h3-4H2,1-2H3
InchiKey: YTQPATWWUJLEJL-UHFFFAOYSA-N
Formula: C5H10ClF2O2PS
SMILES: CCP(=S)(OC)OC(F)(F)CCI
Mol. weight [g/mol]: 238.62

Physical Properties

Property code	Value	Unit	Source
log10ws	1.68		Crippen Method
logp	2.810		Crippen Method
mcvol	145.640	ml/mol	McGowan Method
rinpol	1161.00		NIST Webbook
rinpol	1161.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R544586&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/117-846-3/O-Methyl-O-2-chloro-1-1-difluoroethyl-ethanethionophosphate.pdf>

Generated by Cheméo on 2024-05-05 04:43:08.311335684 +0000 UTC m=+17173437.231912996.

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