Clark 1 propanethio-derivative

Inchi: InChI=1S/C8H16AsClS2/c1-3-7-11-9(5-6-10)12-8-4-2/h5-6H,3-4,7-8H2,1-2H3/b6-5+
InchiKey: JDUUQBFERRKSRF-AATRIKPKSA-N
Formula: C8H16AsClS2
SMILES: CCCS[As](C=CCl)SCCC
Mol. weight [g/mol]: 286.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	4.053		Crippen Method
rinpol	2102.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R514708&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices