O-Ethyl S-nonyl methylphosphonothiolate

Inchi: InChI=1S/C12H27O2PS/c1-4-6-7-8-9-10-11-12-16-15(3,13)14-5-2/h4-12H2,1-3H3
InchiKey: AMXPHGZPXNYMOA-UHFFFAOYSA-N
Formula: C12H27O2PS
SMILES: CCCCCCCCCSP(C)(=O)OCC
Mol. weight [g/mol]: 266.39

Physical Properties

Property code	Value	Unit	Source
hvap	83.42	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.51		Cheméo Relay (1.0)
logp	5.330		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
tb	588.91	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13088896&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature