

4-ethyl-2-hexyl-5-methyl-thiazole

Inchi: InChI=1S/C12H21NS/c1-4-6-7-8-9-12-13-11(5-2)10(3)14-12/h4-9H2,1-3H3
InchiKey: HUPMTZMZEGOTOW-UHFFFAOYSA-N
Formula: C12H21NS
SMILES: CCCCCCc1nc(CC)c(C)s1
Mol. weight [g/mol]: 211.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	4.137		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	1533.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1533.00		NIST Webbook

Sources

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=R497920&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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.chemeo.com/cid/10-036-0/4-ethyl-2-hexyl-5-methyl-thiazole.pdf>

Generated by Cheméo on 2025-12-22 13:08:12.940768334 +0000 UTC m=+6157090.470808999.

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