2-BUTYL-4-ETHYL-5-METHYLTHIAZOLE

Other names: Thiazole, 2-butyl-4-ethyl-5-methyl-
Inchi: InChI=1S/C10H17NS/c1-4-6-7-10-11-9(5-2)8(3)12-10/h4-7H2,1-3H3
InchiKey: CQHWTZNFJRUNPQ-UHFFFAOYSA-N
Formula: C10H17NS
SMILES: CCCCc1nc(CC)c(C)s1
Mol. weight [g/mol]: 183.32

Physical Properties

Property code	Value	Unit	Source
logp	3.357		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinpol	1334.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52414887&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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):

Legend

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.