

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:	CQHWZTNFJRUNPQ-UHFFFAOYSA-N
Formula:	C10H17NS
SMILES:	CCCCc1nc(CC)c(C)s1
Mol. weight [g/mol]:	183.31
CAS:	52414-88-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	3.357		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinpola	1334.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52414887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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