4-Methyl-5-ethylthiazole

Other names:	5-Ethyl-4-methylthiazole
	Thiazole, 5-ethyl-4-methyl-
	5-Ethyl-4-methyl-1,3-thiazole
	Thiazole, 4-methyl-5-ethyl
Inchi:	InChI=1S/C6H9NS/c1-3-6-5(2)7-4-8-6/h4H,3H2,1-2H3
InchiKey:	XPQULTFBJPGINB-UHFFFAOYSA-N
Formula:	C6H9NS
SMILES:	CCc1scnc1C
Mol. weight [g/mol]:	127.21
CAS:	31883-01-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	2.014		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	1004.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1467.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	443.20	K	99.30	NIST Webbook
tbrp	351.70	K	3.30	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=C31883019&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
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure

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