

1H-Pyrrole, 3-ethyl-2,4,5-trimethyl-

Other names:	Pyrrole, 3-ethyl-2,4,5-trimethyl- Phyllopyrrole 2,3,5-Trimethyl-4-ethylpyrrole 3-Ethyl-2,4,5-trimethyl-1H-pyrrole
Inchi:	InChI=1S/C9H15N/c1-5-9-6(2)7(3)10-8(9)4/h10H,5H2,1-4H3
InchiKey:	YEYMBKUFPKCVKT-UHFFFAOYSA-N
Formula:	C9H15N
SMILES:	CCc1c(C)[nH]c(C)c1C
Mol. weight [g/mol]:	137.22
CAS:	520-69-4

Physical Properties

Property code	Value	Unit	Source
chs	-5596.10 ± 5.40	kJ/mol	NIST Webbook
hfs	-89.20 ± 5.40	kJ/mol	NIST Webbook
log10ws	-2.92		Crippen Method
logp	2.020		Crippen Method
mcvol	128.190	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C520694&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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