

1H-Pyrrole, 2,5-diethyl-

Inchi: InChI=1S/C8H13N/c1-3-7-5-6-8(4-2)9-7/h5-6,9H,3-4H2,1-2H3
InchiKey: CIKZQBMEPDKJHF-UHFFFAOYSA-N
Formula: C8H13N
SMILES: CCc1ccc(CC)[nH]1
Mol. weight [g/mol]: 123.20
CAS: 766-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.658		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
tb	459.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	2.30	NIST Webbook

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=C766950&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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