1H-Pyrrole, 2-ethyl-4-methyl-

Other names: 2-ethyl-4-methyl-1H-pyrrole
Inchi: InChI=1S/C7H11N/c1-3-7-4-6(2)5-8-7/h4-5,8H,3H2,1-2H3
InchiKey: GALBJULHRGPJEG-UHFFFAOYSA-N
Formula: C7H11N
SMILES: CCc1cc(C)c[nH]1
Mol. weight [g/mol]: 109.17
CAS: 69687-77-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.404		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	938.00		NIST Webbook
ripol	1711.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69687770&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/25-049-0/1H-Pyrrole-2-ethyl-4-methyl.pdf
Generated by Cheméo on 2024-04-29 03:48:58.1294517 +0000 UTC m=+16651787.050029015.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.