1-Ethyl-1,2,4-triazole

Inchi: InChI=1S/C4H7N3/c1-2-7-4-5-3-6-7/h3-4H,2H2,1H3
InchiKey: FEOIYPLRWRCSMS-UHFFFAOYSA-N
Formula: C4H7N3
SMILES: CCn1cncn1
Mol. weight [g/mol]: 97.12
CAS: 16778-70-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.26		Crippen Method
logp	0.298		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
rinpol	900.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16778704&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.