N-propyl-Tetrahydropyrrole

Other names: 1-Propyl-pyrrolidine
N-propyl-Tetrahydropyrrole
Inchi: InChI=1S/C7H15N/c1-2-5-8-6-3-4-7-8/h2-7H2,1H3
InchiKey: HLNRRPIYRBBHSQ-UHFFFAOYSA-N
Formula: C7H15N
SMILES: CCCN1CCCC1
Mol. weight [g/mol]: 113.20

Physical Properties

Property code	Value	Unit	Source
hvap	40.64	kJ/mol	Cheméo Relay (1.0)
ie	8.07	eV	Cheméo Relay (1.0)
logp	1.492		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
rinpol	857.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	882.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	987.00		NIST Webbook
tb	395.40	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7335071&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature