PIPERIDINE, 1-PROPYL-

Other names:	1-propylpiperidine
	N-Propylpiperidine
	Piperidine, N-propyl-
	Propylpiperidine
Inchi:	InChI=1S/C8H17N/c1-2-6-9-7-4-3-5-8-9/h2-8H2,1H3
InchiKey:	VTDIWMPYBAVEDY-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CCCN1CCCCC1
Mol. weight [g/mol]:	127.23
CAS:	5470-02-0

Physical Properties

Property code	Value	Unit	Source
chl	-5430.60 ± 3.30	kJ/mol	NIST Webbook
hfl	-147.00 ± 3.30	kJ/mol	NIST Webbook
hvap	44.90 ± 0.40	kJ/mol	NIST Webbook
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-0.60		Cheméo Relay (1.0)
logp	1.882		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	930.00		NIST Webbook
ripol	1057.00		NIST Webbook
ripol	1054.00		NIST Webbook
tb	425.25 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.20 ± 0.40	kJ/mol	294.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43127e+01
Coeff. B	-3.54858e+03
Coeff. C	-5.92030e+01
Temperature range (K), min.	312.22
Temperature range (K), max.	453.44

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5470020&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb: Normal Boiling Point Temperature