Propane, 1-isocyano-

Other names:	Propyl isocyanide
	Propylisonitrile
	n-C3H7NC
	n-Propyl isocyanide
Inchi:	InChI=1S/C4H7N/c1-3-4-5-2/h3-4H2,1H3
InchiKey:	FFDKYFGBIQQMSR-UHFFFAOYSA-N
Formula:	C4H7N
SMILES:	[C-]#[N+]CCC
Mol. weight [g/mol]:	69.11
CAS:	627-36-1

Physical Properties

Property code	Value	Unit	Source
affp	856.80	kJ/mol	NIST Webbook
basg	824.30	kJ/mol	NIST Webbook
chl	-2673.00	kJ/mol	NIST Webbook
gf	115.98	kJ/mol	Joback Method
hf	38.99	kJ/mol	Joback Method
hfus	7.62	kJ/mol	Joback Method
hvap	34.98	kJ/mol	Joback Method
ie	11.33	eV	NIST Webbook
ie	11.80 ± 0.25	eV	NIST Webbook
ie	11.10 ± 0.10	eV	NIST Webbook
log10ws	-3.26		Crippen Method
logp	1.316		Crippen Method
mcvol	68.600	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
tb	393.00	K	Joback Method
tc	585.13	K	Joback Method
tf	199.83	K	Joback Method
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.15	J/mol×K	393.00	Joback Method
cpg	124.57	J/mol×K	425.02	Joback Method
cpg	130.74	J/mol×K	457.04	Joback Method
cpg	136.66	J/mol×K	489.07	Joback Method
cpg	142.33	J/mol×K	521.09	Joback Method
cpg	147.77	J/mol×K	553.11	Joback Method
cpg	152.98	J/mol×K	585.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35303e+01
Coeff. B	-3.08704e+03
Coeff. C	-4.46080e+01
Temperature range (K), min.	277.72
Temperature range (K), max.	420.21

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627361&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

affp: Proton affinity

basg: Gas basicity

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume