Propane, 1-isocyanato-

Other names:	1-Isocyanatopropane
	1-Propyl isocyanate
	Isocyanic acid n-propyl ester
	Isocyanic acid, propyl ester
	Propyl isocyanate
	UN 2482
	n-Propyl isocyanate
Inchi:	InChI=1S/C4H7NO/c1-2-3-5-4-6/h2-3H2,1H3
InchiKey:	OQURWGJAWSLGQG-UHFFFAOYSA-N
Formula:	C4H7NO
SMILES:	CCCN=C=O
Mol. weight [g/mol]:	85.10
CAS:	110-78-1

Physical Properties

Property code	Value	Unit	Source
hf	-131.30	kJ/mol	Joback Method
hvap	34.03	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	0.732		Crippen Method
mcvol	74.470	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	357.59	K	Joback Method
tc	536.84	K	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43542e+01
Coeff. B	-3.20748e+03
Coeff. C	-4.02990e+01
Temperature range (K), min.	268.32

Temperature range (K), max.	395.00

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110781&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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