Propane, 1-isocyanato-2-methyl-

Other names:	2-methylpropyl isocyanate
	Isobutyl isocyanate
	Isocyanic acid, isobutyl ester
	UN 2486
Inchi:	InChI=1S/C5H9NO/c1-5(2)3-6-4-7/h5H,3H2,1-2H3
InchiKey:	NNZVKALEGZPYKL-UHFFFAOYSA-N
Formula:	C5H9NO
SMILES:	CC(C)CN=C=O
Mol. weight [g/mol]:	99.13
CAS:	1873-29-6

Physical Properties

Property code	Value	Unit	Source
hf	-157.22	kJ/mol	Joback Method
hvap	35.87	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	0.978		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	380.03	K	Joback Method
tc	563.03	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	44.20	kJ/mol	324.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.03333e+01
Coeff. B	-2.01292e+03
Coeff. C	-4.65540e+01
Temperature range (K), min.	246.93
Temperature range (K), max.	447.39

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1873296&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

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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