Propane, 2-isocyano-2-methyl-

Other names:	(CH3)3CNC
	2-Methyl-2-isocyanopropane
	2-methylpropyl isocyanide
	TBIN
	t-Butyl isocyanide
	tert-Butyl Isocyanide
	tert-Butylisonitrile
Inchi:	InChI=1S/C5H9N/c1-5(2,3)6-4/h1-3H3
InchiKey:	FAGLEPBREOXSAC-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	[C-]#[N+]C(C)(C)C
Mol. weight [g/mol]:	83.13
CAS:	7188-38-7

Physical Properties

Property code	Value	Unit	Source
affp	870.70	kJ/mol	NIST Webbook
basg	838.30	kJ/mol	NIST Webbook
gf	127.24	kJ/mol	Joback Method
hf	9.60	kJ/mol	Joback Method
hfus	2.80	kJ/mol	Joback Method
hvap	35.91	kJ/mol	Joback Method
ie	10.50	eV	NIST Webbook
log10ws	-3.79		Crippen Method
logp	1.704		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	365.00	K	NIST Webbook
tc	616.42	K	Joback Method
tf	282.15 ± 4.00	K	NIST Webbook
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.24	J/mol×K	412.65	Joback Method
cpg	164.35	J/mol×K	446.61	Joback Method
cpg	172.92	J/mol×K	480.57	Joback Method
cpg	180.97	J/mol×K	514.54	Joback Method
cpg	188.53	J/mol×K	548.50	Joback Method
cpg	195.62	J/mol×K	582.46	Joback Method
cpg	202.27	J/mol×K	616.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52593e+01
Coeff. B	-3.43148e+03
Coeff. C	-4.25230e+01
Temperature range (K), min.	271.72
Temperature range (K), max.	387.47

Sources

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=C7188387&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

Legend

affp: Proton affinity

basg: Gas basicity

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