Butane, 1-isocyanato-

Other names:	1-Butyl isocyanate
	1-Isocyanatobutane
	BIC
	Butyl isocyanate
	Isocyanic acid n-butyl ester
	Isocyanic acid, butyl ester
	UN 2485
	n-Butyl isocyanate
	n-C4H9NCO
Inchi:	InChI=1S/C5H9NO/c1-2-3-4-6-5-7/h2-4H2,1H3
InchiKey:	HNHVTXYLRVGMHD-UHFFFAOYSA-N
Formula:	C5H9NO
SMILES:	CCCCN=C=O
Mol. weight [g/mol]:	99.13
CAS:	111-36-4

Physical Properties

Property code	Value	Unit	Source
hf	-151.94	kJ/mol	Joback Method
hvap	36.26	kJ/mol	Joback Method
ie	10.14 ± 0.05	eV	NIST Webbook
log10ws	-5.41		Crippen Method
logp	1.122		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
tb	388.00 ± 4.00	K	NIST Webbook
tc	559.17	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	38.50	kJ/mol	340.50	NIST Webbook
hvapt	46.80	kJ/mol	331.00	NIST Webbook

pvap	2.48	kPa	294.15	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	9.52	kPa	323.24	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	17.88	kPa	338.02	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	32.10	kPa	353.02	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	44.82	kPa	362.65	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	61.84	kPa	372.60	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K
pvap	99.08	kPa	387.87	Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58634e+01
Coeff. B	-3.81145e+03
Coeff. C	-4.90560e+01
Temperature range (K), min.	293.76
Temperature range (K), max.	410.26

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor-Liquid Equilibrium Studies for Systems Containing n-Butylisocyanate at Temperatures between 323.15 K and 371.15 K:	https://www.doi.org/10.1021/je030222n
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=C111364&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hf:	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
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature