

Butane, 1-isocyano-

Other names:	Butyl isocyanide Butylisonitrile n-Butyl isocyanide n-C4H9NC
Inchi:	InChI=1S/C5H9N/c1-3-4-5-6-2/h3-5H2,1H3
InchiKey:	FSBLVBBRXSCOKU-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	[C-]#[N+]CCCC
Mol. weight [g/mol]:	83.13
CAS:	2769-64-4

Physical Properties

Property code	Value	Unit	Source
gf	124.40	kJ/mol	Joback Method
hf	18.35	kJ/mol	Joback Method
hfus	10.21	kJ/mol	Joback Method
hvap	37.20	kJ/mol	Joback Method
ie	11.71 ± 0.05	eV	NIST Webbook
ie	11.10	eV	NIST Webbook
log10ws	-3.68		Crippen Method
logp	1.706		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	415.88	K	Joback Method
tc	606.51	K	Joback Method
tf	211.10	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.81	J/mol×K	415.88	Joback Method
cpg	160.74	J/mol×K	447.65	Joback Method
cpg	168.35	J/mol×K	479.42	Joback Method

cpg	175.64	J/mol×K	511.20	Joback Method
cpg	182.62	J/mol×K	542.97	Joback Method
cpg	189.29	J/mol×K	574.74	Joback Method
cpg	195.68	J/mol×K	606.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61825e+01
Coeff. B	-3.91686e+03
Coeff. C	-5.16970e+01
Temperature range (K), min.	298.12
Temperature range (K), max.	412.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2769644&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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