Butanenitrile, 2-methyl-

Other names:	2-Cyanobutane
	2-Methylbutanenitrile
	2-Methylbutylnitrile
	2-Methylbutyronitrile
	Butyronitrile, 2-methyl-
	«alpha»-Methylbutyronitrile
	Â«alphaÂ»-Methylbutyronitrile
Inchi:	InChI=1S/C5H9N/c1-3-5(2)4-6/h5H,3H2,1-2H3
InchiKey:	RCEJCSULJQNRQQ-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	CCC(C)C#N
Mol. weight [g/mol]:	83.13
CAS:	18936-17-9

Physical Properties

Property code	Value	Unit	Source
chl	-3213.80 ± 1.40	kJ/mol	NIST Webbook
gf	121.96	kJ/mol	Joback Method
hf	2.40 ± 1.40	kJ/mol	NIST Webbook
hfl	-40.03	kJ/mol	NIST Webbook
hfus	6.69	kJ/mol	Joback Method
hvap	42.47 ± 0.29	kJ/mol	NIST Webbook
hvap	42.40	kJ/mol	NIST Webbook
hvap	40.60 ± 0.06	kJ/mol	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.556		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	729.00		NIST Webbook
rinpol	717.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1091.00		NIST Webbook
tb	399.70 ± 3.00	K	NIST Webbook
tb	398.00 ± 4.00	K	NIST Webbook
tb	398.70 ± 3.00	K	NIST Webbook
tb	398.20	K	NIST Webbook

tb	400.00 ± 3.00	K	NIST Webbook
tb	396.00 ± 3.00	K	NIST Webbook
tb	397.00 ± 3.00	K	NIST Webbook
tb	398.00 ± 1.00	K	NIST Webbook
tb	398.00 ± 3.00	K	NIST Webbook
tb	399.00 ± 0.50	K	NIST Webbook
tc	610.63	K	Joback Method
tf	196.10	K	Joback Method
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.56	J/mol×K	578.10	Joback Method
cpg	152.89	J/mol×K	415.44	Joback Method
cpg	161.10	J/mol×K	447.97	Joback Method
cpg	168.97	J/mol×K	480.50	Joback Method
cpg	176.49	J/mol×K	513.03	Joback Method
cpg	183.69	J/mol×K	545.56	Joback Method
cpg	197.11	J/mol×K	610.63	Joback Method
hvapt	42.50 ± 0.30	kJ/mol	293.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18936179&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

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume