

2-METHYLBUTYRONITRILE

Other names:	2-Cyanobutane 2-Methylbutanenitrile 2-Methylbutylnitrile Butyronitrile, 2-methyl- «alpha»-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
hf	2.40 ± 1.40	kJ/mol	NIST Webbook
hfl	-40.03	kJ/mol	NIST Webbook
hfus	6.69	kJ/mol	Joback Method
hvap	40.60 ± 0.06	kJ/mol	NIST Webbook
hvap	42.40	kJ/mol	NIST Webbook
hvap	42.47 ± 0.29	kJ/mol	NIST Webbook
ie	11.06	eV	Cheméo Relay (1.0)
logp	1.556		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
rinpol	717.00		NIST Webbook
rinpol	729.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1094.00		NIST Webbook
tb	398.00 ± 1.00	K	NIST Webbook
tb	398.70 ± 3.00	K	NIST Webbook
tb	398.00 ± 4.00	K	NIST Webbook
tb	400.00 ± 3.00	K	NIST Webbook
tb	399.00 ± 0.50	K	NIST Webbook
tb	397.00 ± 3.00	K	NIST Webbook
tb	398.20	K	NIST Webbook
tb	398.00 ± 3.00	K	NIST Webbook

tb	399.70 ± 3.00	K	NIST Webbook
tb	396.00 ± 3.00	K	NIST Webbook
tf	195.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	190.56	J/mol×K	578.10	Joback Method
cpg	197.11	J/mol×K	610.63	Joback Method
hvapt	42.50 ± 0.30	kJ/mol	293.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39063e+01
Coeff. B	-2.82768e+03
Coeff. C	-9.35540e+01
Temperature range (K), min.	301.19
Temperature range (K), max.	422.55

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C18936179&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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