ISOVALERONITRILE

Other names:	1-Cyano-2-methylpropane
	2-Methylbutane secondary mononitrile
	3-Methylbutanenitrile
	3-Methylbutylnitrile
	3-Methylbutyronitrile
	Butyronitrile, 3-methyl-
	Isoamylnitrile
	Isobutyl cyanide
	Isopentane nitrile
	NSC 148363
	iso-C4H9CN
Inchi:	InChI=1S/C5H9N/c1-5(2)3-4-6/h5H,3H2,1-2H3
InchiKey:	QHDRKFYEGYYIIK-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	CC(C)CC#N
Mol. weight [g/mol]:	83.13
CAS:	625-28-5

Physical Properties

Property code	Value	Unit	Source
chl	-3246.00	kJ/mol	NIST Webbook
ea	0.01 ± 0.00	eV	NIST Webbook
hf	5.29	kJ/mol	Cheméo Relay (1.0)
hfus	6.69	kJ/mol	Joback Method
hvap	41.69	kJ/mol	NIST Webbook
hvap	41.64 ± 0.03	kJ/mol	NIST Webbook
ie	11.25	eV	Cheméo Relay (1.0)
log10ws	-1.28		Cheméo Relay (1.0)
logp	1.556		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	730.40		NIST Webbook
rinpol	730.40		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	731.00		NIST Webbook
ripol	1134.00		NIST Webbook

ripol	1090.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1125.00		NIST Webbook
tb	402.00 ± 3.00	K	NIST Webbook
tb	402.70 ± 3.00	K	NIST Webbook
tb	400.00 ± 3.00	K	NIST Webbook
tb	401.70 ± 3.00	K	NIST Webbook
tb	398.00 ± 5.00	K	NIST Webbook
tb	402.00 ± 3.00	K	NIST Webbook
tb	403.70 ± 2.00	K	NIST Webbook
tb	402.00 ± 3.00	K	NIST Webbook
tb	401.00 ± 3.00	K	NIST Webbook
tb	400.60	K	NIST Webbook
tf	172.30 ± 0.30	K	NIST Webbook
tf	172.30 ± 0.50	K	NIST Webbook
vc	0.307	m3/kmol	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	35.10	kJ/mol	400.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	402.20	K	97.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41046e+01
Coeff. B	-2.90302e+03
Coeff. C	-9.49780e+01
Temperature range (K), min.	305.08
Temperature range (K), max.	425.12

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625285&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

Cheméo Relay (1.0):

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

ea: Electron affinity

hf: 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

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point
vc:	Critical Volume