Isobutyronitrile

Other names:	Propanenitrile, 2-methyl-
	Isopropyl cyanide
	Isopropylnitrile
	1-Cyano-1-methylethane
	2-Cyanopropane
	2-Methylpropanenitrile
	2-Methylpropionitrile
	iso-C3H7CN
	Dimethylacetonitrile
	Isopropylkyanid
	UN 2284
	«alpha»-Methylpropanenitrile
	NSC 60536
Inchi:	InChI=1S/C4H7N/c1-4(2)3-5/h4H,1-2H3
InchiKey:	LRDFRRGEGBBSRN-UHFFFAOYSA-N
Formula:	C4H7N
SMILES:	CC(C)C#N
Mol. weight [g/mol]:	69.11
CAS:	78-82-0

Physical Properties

Property code	Value	Unit	Source
affp	803.60	kJ/mol	NIST Webbook
basg	772.80	kJ/mol	NIST Webbook
chl	-2562.30 ± 0.75	kJ/mol	NIST Webbook
chl	-2560.60 ± 1.30	kJ/mol	NIST Webbook
ea	0.01 ± 0.00	eV	NIST Webbook
gf	113.54	kJ/mol	Joback Method
hf	22.80	kJ/mol	NIST Webbook
hf	24.30 ± 1.80	kJ/mol	NIST Webbook
hfl	-12.20 ± 0.84	kJ/mol	NIST Webbook
hfl	-13.80	kJ/mol	NIST Webbook
hfus	4.10	kJ/mol	Joback Method
hvap	37.13 ± 0.02	kJ/mol	NIST Webbook
hvap	37.22	kJ/mol	NIST Webbook
hvap	36.70	kJ/mol	NIST Webbook
hvap	36.60	kJ/mol	NIST Webbook

hvap	36.50	kJ/mol	NIST Webbook
ie	11.74	eV	NIST Webbook
ie	11.74	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.166		Crippen Method
mcvol	68.600	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	590.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	637.20		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	594.40		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	626.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	993.00		NIST Webbook
ripol	1009.00		NIST Webbook
tb	377.00 ± 0.30	K	NIST Webbook
tb	381.00 ± 5.00	K	NIST Webbook
tb	380.00 ± 5.00	K	NIST Webbook
tb	377.00	K	NIST Webbook
tb	380.70	K	NIST Webbook
tb	376.40 ± 2.00	K	NIST Webbook
tb	380.70 ± 6.00	K	NIST Webbook
tb	376.90 ± 0.50	K	NIST Webbook
tb	381.00 ± 4.00	K	NIST Webbook
tb	376.50 ± 3.00	K	NIST Webbook
tb	374.70 ± 1.00	K	NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tb	376.70 ± 2.00	K	NIST Webbook
tb	375.00 ± 3.00	K	NIST Webbook
tb	374.70 ± 3.00	K	NIST Webbook
tb	376.70 ± 7.00	K	NIST Webbook
tb	374.70 ± 1.50	K	NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tb	382.00 ± 5.00	K	NIST Webbook
tc	589.40	K	Joback Method
tf	201.65 ± 0.50	K	NIST Webbook
tf	201.65 ± 0.50	K	NIST Webbook
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.40	J/mol×K	490.98	Joback Method
cpg	143.27	J/mol×K	523.79	Joback Method
cpg	148.89	J/mol×K	556.60	Joback Method
cpg	118.18	J/mol×K	392.56	Joback Method
cpg	124.86	J/mol×K	425.37	Joback Method
cpg	131.27	J/mol×K	458.17	Joback Method
cpg	154.25	J/mol×K	589.40	Joback Method
cpl	156.20	J/mol×K	297.00	NIST Webbook
hvapt	32.39	kJ/mol	377.00	NIST Webbook
hvapt	35.90	kJ/mol	339.00	NIST Webbook
hvapt	37.50	kJ/mol	327.50	NIST Webbook

Sources

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=C78820&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
ea: Electron affinity
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
ie:	Ionization energy
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