Propanenitrile, 2,2-dimethyl-

Other names:	(CH3)3C-CN
	2,2-Dimethylpropanenitrile
	2,2-Dimethylpropionitrile
	2-Cyano-2-methylpropane
	NSC 890
	Pivalonitrile
	Trimethylacetonitrile
	tert-Butyl cyanide
	tert-Butylnitrile
Inchi:	InChI=1S/C5H9N/c1-5(2,3)4-6/h1-3H3
InchiKey:	JAMNHZBIQDNHMM-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	CC(C)(C)C#N
Mol. weight [g/mol]:	83.13
CAS:	630-18-2

Physical Properties

Property code	Value	Unit	Source
affp	810.90	kJ/mol	NIST Webbook
basg	780.20	kJ/mol	NIST Webbook
chl	-3213.90 ± 0.71	kJ/mol	NIST Webbook
ea	0.01 ± 0.00	eV	NIST Webbook
gf	127.24	kJ/mol	Joback Method
hf	-3.30	kJ/mol	NIST Webbook
hfl	-39.90	kJ/mol	NIST Webbook
hfus	2.80	kJ/mol	Joback Method
hvap	36.60	kJ/mol	NIST Webbook
hvap	37.35 ± 0.03	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
hvap	37.50	kJ/mol	NIST Webbook
hvap	36.70	kJ/mol	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.556		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
sl	232.00	J/mol×K	NIST Webbook
tb	412.65	K	Joback Method

tc	616.42	K	Joback Method
tf	288.65 ± 2.00	K	NIST Webbook
tt	292.13 ± 0.02	K	NIST Webbook
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.27	J/mol×K	616.42	Joback Method
cpg	155.24	J/mol×K	412.65	Joback Method
cpg	195.62	J/mol×K	582.46	Joback Method
cpg	188.53	J/mol×K	548.50	Joback Method
cpg	180.97	J/mol×K	514.54	Joback Method
cpg	172.92	J/mol×K	480.57	Joback Method
cpg	164.35	J/mol×K	446.61	Joback Method
cpl	179.37	J/mol×K	298.15	NIST Webbook
cpl	153.30	J/mol×K	297.00	NIST Webbook
hfust	1.91	kJ/mol	232.70	NIST Webbook
hfust	0.23	kJ/mol	213.00	NIST Webbook
hfust	9.29	kJ/mol	292.10	NIST Webbook
hfust	9.29	kJ/mol	292.10	NIST Webbook
hvapt	36.50	kJ/mol	342.00	NIST Webbook
hvapt	32.40	kJ/mol	379.20	NIST Webbook
hvapt	37.00	kJ/mol	332.00	NIST Webbook
sfust	7.78	J/mol×K	232.70	NIST Webbook
sfust	31.80	J/mol×K	292.10	NIST Webbook
sfust	1.09	J/mol×K	213.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56833e+01
Coeff. B	-3.69387e+03
Coeff. C	-3.61660e+01
Temperature range (K), min.	276.09
Temperature range (K), max.	392.31

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630182&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

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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume