

Acetyl cyanide

Other names:	Pyruvonitrile
	Propanenitrile, 2-oxo-
	«alpha»-Oxopropionitrile
	Oxopropionitrile
	Oxypropionitrile
	Pyruvic acid nitrile
	2-Oxopropionitrile
	CH ₃ C(O)CN
	2-Oxopropanenitrile
	2-Oxopropiononitrile
Inchi:	InChI=1S/C3H3NO/c1-3(5)2-4/h1H3
InchiKey:	QLDHWVVRQCGZLE-UHFFFAOYSA-N
Formula:	C ₃ H ₃ NO
SMILES:	CC(=O)C#N
Mol. weight [g/mol]:	69.06
CAS:	631-57-2

Physical Properties

Property code	Value	Unit	Source
affp	746.90	kJ/mol	NIST Webbook
basg	716.20	kJ/mol	NIST Webbook
gf	-21.36	kJ/mol	Joback Method
hf	-52.95	kJ/mol	Joback Method
hfus	6.63	kJ/mol	Joback Method
hvap	39.50	kJ/mol	Joback Method
log10ws	-0.23		Crippen Method
logp	0.099		Crippen Method
mcvol	56.080	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
tb	365.50	K	NIST Webbook
tc	631.13	K	Joback Method
tf	238.49	K	Joback Method
vc	0.235	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.03	J/mol×K	423.99	Joback Method
cpg	96.24	J/mol×K	458.51	Joback Method
cpg	100.26	J/mol×K	493.04	Joback Method
cpg	104.10	J/mol×K	527.56	Joback Method
cpg	107.76	J/mol×K	562.08	Joback Method
cpg	111.25	J/mol×K	596.60	Joback Method
cpg	114.55	J/mol×K	631.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C631572&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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