

1-Cyanoethyl radical

Inchi:	InChI=1S/C3H4N/c1-2-3-4/h2H,1H3
InchiKey:	VQGISNOMGHCEPX-UHFFFAOYSA-N
Formula:	C3H4N
SMILES:	C[CH]C#N
Mol. weight [g/mol]:	54.07
CAS:	3264-99-1

Physical Properties

Property code	Value	Unit	Source
ea	1.77 ± 0.01	eV	NIST Webbook
ea	1.50 ± 0.10	eV	NIST Webbook
gf	157.50	kJ/mol	Joback Method
hf	110.16	kJ/mol	Joback Method
hfus	3.19	kJ/mol	Joback Method
hvap	32.22	kJ/mol	Joback Method
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.734		Crippen Method
mcvol	52.360	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	368.98	K	Joback Method
tc	563.43	K	Joback Method
tf	189.93	K	Joback Method
vc	0.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	80.71	J/mol×K	368.98	Joback Method
cpg	85.35	J/mol×K	401.39	Joback Method
cpg	89.64	J/mol×K	433.80	Joback Method
cpg	93.60	J/mol×K	466.21	Joback Method
cpg	97.27	J/mol×K	498.61	Joback Method
cpg	100.66	J/mol×K	531.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3264991&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
ie:	Ionization energy
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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