2-Cyanoethyl radical

Inchi: InChI=1S/C3H4N/c1-2-3-4/h1-2H2
InchiKey: WEMXRTXQKRXSIO-UHFFFAOYSA-N
Formula: C3H4N
SMILES: [CH2]CC#N
Mol. weight [g/mol]: 54.07
CAS: 25840-11-3

Physical Properties

Property code	Value	Unit	Source
ea	1.24 ± 0.10	eV	NIST Webbook
gf	159.94	kJ/mol	Joback Method
hf	115.44	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	32.60	kJ/mol	Joback Method
ie	9.90 ± 0.10	eV	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.734		Crippen Method
mcvol	52.360	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	369.42	K	Joback Method
tc	559.13	K	Joback Method
tf	204.93	K	Joback Method
vc	0.221	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	80.74	J/mol×K	369.42	Joback Method
cpg	85.16	J/mol×K	401.04	Joback Method
cpg	89.26	J/mol×K	432.66	Joback Method
cpg	93.05	J/mol×K	464.28	Joback Method
cpg	96.56	J/mol×K	495.89	Joback Method
cpg	99.83	J/mol×K	527.51	Joback Method
cpg	102.86	J/mol×K	559.13	Joback Method

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=C25840113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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