

Ethyl isocyanide

Other names:	Ethyl carbylamine Ethane, isocyano- Isocyanoethane C2H5NC Carbylamine, ethyl- Ethylisokyanid Ethylkarbylamin Ethyl isonitrile
Inchi:	InChI=1S/C3H5N/c1-3-4-2/h3H2,1H3
InchiKey:	BPCWCZCOOFUXGQ-UHFFFAOYSA-N
Formula:	C3H5N
SMILES:	[C-]#[N+]CC
Mol. weight [g/mol]:	55.08
CAS:	624-79-3

Physical Properties

Property code	Value	Unit	Source
affp	851.30	kJ/mol	NIST Webbook
basg	818.90	kJ/mol	NIST Webbook
chl	-2005.00	kJ/mol	NIST Webbook
chl	-2005.00	kJ/mol	NIST Webbook
gf	107.56	kJ/mol	Joback Method
hf	132.60	kJ/mol	NIST Webbook
hfl	99.60	kJ/mol	NIST Webbook
hfus	5.03	kJ/mol	Joback Method
hvap	33.00	kJ/mol	NIST Webbook
ie	11.20 ± 0.10	eV	NIST Webbook
ie	11.20 ± 0.25	eV	NIST Webbook
ie	11.38	eV	NIST Webbook
log10ws	-2.84		Crippen Method
logp	0.926		Crippen Method
mcvol	54.510	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	370.12	K	Joback Method
tc	563.45	K	Joback Method
tf	188.56	K	Joback Method
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.00	J/mol×K	370.12	Joback Method
cpg	90.77	J/mol×K	402.34	Joback Method
cpg	95.36	J/mol×K	434.56	Joback Method
cpg	99.78	J/mol×K	466.78	Joback Method
cpg	104.02	J/mol×K	499.00	Joback Method
cpg	108.09	J/mol×K	531.23	Joback Method
cpg	112.00	J/mol×K	563.45	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=C624793&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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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