Isocyanic acid

Inchi: InChI=1S/CHNO/c2-1-3/h2H
InchiKey: OWIKHYCFFJSOEH-UHFFFAOYSA-N
Formula: CHNO
SMILES: N=C=O
Mol. weight [g/mol]: 43.02
CAS: 75-13-8

Physical Properties

Property code	Value	Unit	Source
affp	753.00	kJ/mol	NIST Webbook
basg	718.80	kJ/mol	NIST Webbook
gf	59.41	kJ/mol	Joback Method
hf	-97.00 ± 13.00	kJ/mol	NIST Webbook
hvap	36.04	kJ/mol	Joback Method
ie	11.62 ± 0.02	eV	NIST Webbook
ie	11.60 ± 0.01	eV	NIST Webbook
ie	11.60 ± 0.01	eV	NIST Webbook
ie	11.60 ± 0.01	eV	NIST Webbook
log10ws	-5.49		Crippen Method
logp	-0.099		Crippen Method
mcvol	32.200	ml/mol	McGowan Method
tb	296.73	K	Joback Method
tf	211.27	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	40.50	J/mol×K	296.73	Joback Method
cpg	17.53	J/mol×K	100.12	Joback Method
cpg	17.53	J/mol×K	100.12	Joback Method
cpg	17.53	J/mol×K	100.12	Joback Method
cpg	17.53	J/mol×K	100.12	Joback Method
cpg	17.53	J/mol×K	100.12	Joback Method
cpg	17.53	J/mol×K	100.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75138&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

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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point