CYANIC ACID

Inchi: InChI=1S/CH5NO/c2-1-3/h3H,1-2H2
InchiKey: XMYQHJDBLRZMLW-UHFFFAOYSA-N
Formula: CH5NO
SMILES: NCO
Mol. weight [g/mol]: 43.02
CAS: 420-05-3

Physical Properties

Property code	Value	Unit	Source
hf	-177.23	kJ/mol	Cheméo Relay (1.0)
hfus	7.63	kJ/mol	Joback Method
ie	10.16	eV	Cheméo Relay (1.0)
log10ws	1.75		Cheméo Relay (1.0)
logp	-1.105		Crippen Method
mcvol	40.800	ml/mol	McGowan Method
pc	7367.98	kPa	Joback Method
tb	419.90	K	Cheméo Relay (1.0)
tc	640.25	K	Cheméo Relay (1.0)
tf	330.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.72	J/mol×K	386.99	Joback Method
cpg	78.34	J/mol×K	416.87	Joback Method
cpg	81.82	J/mol×K	446.74	Joback Method
cpg	85.17	J/mol×K	476.62	Joback Method
cpg	88.39	J/mol×K	506.49	Joback Method
cpg	91.47	J/mol×K	536.37	Joback Method
cpg	94.44	J/mol×K	566.24	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1455.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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