

Cyanic acid

Inchi:	InChI=1S/CHNO/c2-1-3/h3H
InchiKey:	XLJMAIOERFSOGZ-UHFFFAOYSA-N
Formula:	CHNO
SMILES:	N#CO
Mol. weight [g/mol]:	43.02
CAS:	420-05-3

Physical Properties

Property code	Value	Unit	Source
af	0.5071		Cheméo Relay (1.0)
ea	0.67 ± 0.03	eV	NIST Webbook
gf	-46.10	kJ/mol	Joback Method
hf	-99.11	kJ/mol	Cheméo Relay (1.0)
hfus	3.94	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Cheméo Relay (1.0)
ie	11.26	eV	Cheméo Relay (1.0)
logp	-0.160		Crippen Method
mcvol	32.200	ml/mol	McGowan Method
pc	6430.83	kPa	Joback Method
tb	394.63	K	Cheméo Relay (1.0)
tc	599.22	K	Cheméo Relay (1.0)
tf	304.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	47.53	J/mol×K	416.54	Joback Method
cpg	48.91	J/mol×K	448.01	Joback Method
cpg	50.25	J/mol×K	479.49	Joback Method
cpg	51.54	J/mol×K	510.96	Joback Method
cpg	52.78	J/mol×K	542.43	Joback Method
cpg	53.98	J/mol×K	573.90	Joback Method
cpg	55.13	J/mol×K	605.38	Joback Method
hvapt	30.70	kJ/mol	250.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53676e+01
Coeff. B	-2.87137e+03
Coeff. C	-2.93580e+01
Temperature range (K), min.	219.77
Temperature range (K), max.	314.89

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C420053&Units=SI>

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):

Legend

af:	Acentric Factor
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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