Propanenitrile, 3-hydroxy-

Other names:	1-Cyano-2-hydroxyethane
	2-Cyano-1-ethanol
	2-Cyanoethanol
	2-Cyanoethyl alcohol
	2-Hydroxycyanoethane
	2-Hydroxyethyl cyanide
	2-Hydroxyethylkyanid
	3-Hydroxyacrylonitrile
	3-Hydroxypropanenitrile
	3-Hydroxypropionitrile
	3-hydroxypropiononitrile
	Ethylene cyanohydrin
	Glycol cyanohydrin
	Hydracrylonitrile
	Hydroxypropanenitrile
	Methanolacetonitrile
	NSC 2598
	Propionitrile, 3-hydroxy-
	USAF RH-7
	beta-Hpn
	beta-Hpn3
	«beta»-Cyanoethanol
	«beta»-Hydroxypropionitrile
	Â«betaÂ»-Cyanoethanol
	Â«betaÂ»-Hydroxypropionitrile
Inchi:	InChI=1S/C3H5NO/c4-2-1-3-5/h5H,1,3H2
InchiKey:	WSGYTJNNHPZFKR-UHFFFAOYSA-N
Formula:	C3H5NO
SMILES:	N#CCCO
Mol. weight [g/mol]:	71.08
CAS:	109-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-29.26	kJ/mol	Joback Method
hf	-92.60	kJ/mol	Joback Method

hfus	9.12	kJ/mol	Joback Method
hvap	62.30 ± 0.50	kJ/mol	NIST Webbook
log10ws	-0.21		Crippen Method
logp	-0.108		Crippen Method
mcvol	60.380	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
tb	502.85	K	NIST Webbook
tb	501.20	K	NIST Webbook
tc	647.69	K	Joback Method
tf	226.95	K	NIST Webbook
vc	0.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.10	J/mol×K	493.20	Joback Method
cpg	138.68	J/mol×K	647.69	Joback Method
cpg	135.10	J/mol×K	616.79	Joback Method
cpg	131.36	J/mol×K	585.89	Joback Method
cpg	127.45	J/mol×K	555.00	Joback Method
cpg	123.36	J/mol×K	524.10	Joback Method
cpg	114.64	J/mol×K	462.30	Joback Method
hvapt	53.40	kJ/mol	412.50	NIST Webbook
pvap	0.14	kPa	338.50	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.06	kPa	326.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.08	kPa	328.60	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.09	kPa	331.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.09	kPa	331.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile

pvap	0.11	kPa	333.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.13	kPa	336.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.12	kPa	336.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.06	kPa	325.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.16	kPa	340.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.18	kPa	341.50	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.20	kPa	343.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.26	kPa	346.60	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.34	kPa	351.70	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.44	kPa	356.80	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.58	kPa	361.80	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.05	kPa	323.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile

pvap	0.05	kPa	321.70	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.05	kPa	321.40	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.04	kPa	318.60	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.04	kPa	317.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.03	kPa	314.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.02	kPa	311.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile
pvap	0.02	kPa	306.30	Experimental and computational thermochemical study of 3-hydroxypropanenitrile

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.00 ± 1.00	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.79216e+01
Coeff. B	-6.94952e+03

Coeff. C	2.11910e+01
Temperature range (K), min.	372.91
Temperature range (K), max.	529.91

Sources

Experimental and computational thermochemical study of 3-hydroxypropanenitrile:	https://www.doi.org/10.1016/j.jct.2007.03.011
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=C109784&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume