

Propanenitrile, 2-hydroxy-

Other names:	2-HYDROXYPROPIONITRILE 2-Hydroxypropanenitrile 2-Hydroxypropannitril ACETALDEHYDE ALPHA-HYDROXYPROPIONITRILE Acetaldehyde, cyanohydrin Acetocyanohydrin CYANOHYDRIN LACTONITRILE Laktonitril NSC 7764 Propionitrile, 2-hydroxy- «alpha»-Hydroxypropionitrile Â«alphaÂ»-Hydroxypropionitrile
Inchi:	InChI=1S/C3H5NO/c1-3(5)2-4/h3,5H,1H3
InchiKey:	WOFDVFDFSGLBFAC-UHFFFAOYSA-N
Formula:	C3H5NO
SMILES:	CC(O)C#N
Mol. weight [g/mol]:	71.08
CAS:	78-97-7

Physical Properties

Property code	Value	Unit	Source
gf	-31.70	kJ/mol	Joback Method
hf	-97.88	kJ/mol	Joback Method
hfus	5.60	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	-0.109		Crippen Method
mcvol	60.380	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	461.86	K	Joback Method
tc	651.40	K	Joback Method
tf	233.15 ± 0.50	K	NIST Webbook
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.90	J/mol×K	461.86	Joback Method
cpg	119.53	J/mol×K	493.45	Joback Method
cpg	123.96	J/mol×K	525.04	Joback Method
cpg	128.20	J/mol×K	556.63	Joback Method
cpg	132.24	J/mol×K	588.22	Joback Method
cpg	136.10	J/mol×K	619.81	Joback Method
cpg	139.77	J/mol×K	651.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	6.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	3.35615e+01
Coeff. B	-9.34973e+03
Coeff. C	-7.41150e+01
Temperature range (K), min.	355.11
Temperature range (K), max.	405.08

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1402

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78977&Units=SI>
The Yaws Handbook of Vapor Pressure: <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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
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

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