hydrogen peroxide

Other names: ALBONE
DIHYDROGEN DIOXIDE
Inchi: InChI=1S/H2O2/c1-2/h1-2H
InchiKey: MHAJPDPJQMAIIY-UHFFFAOYSA-N
Formula: H2O2
SMILES: OO
Mol. weight [g/mol]: 34.01
CAS: 7722-84-1

Physical Properties

Property code	Value	Unit	Source
affp	674.50	kJ/mol	NIST Webbook
basg	643.80	kJ/mol	NIST Webbook
gf	-324.52	kJ/mol	Joback Method
hf	-347.79	kJ/mol	Joback Method
hfus	3.93	kJ/mol	Joback Method
hvap	48.95	kJ/mol	Joback Method
ie	10.92 ± 0.05	eV	NIST Webbook
ie	11.70	eV	NIST Webbook
ie	11.69	eV	NIST Webbook
ie	11.26 ± 0.05	eV	NIST Webbook
ie	10.58 ± 0.04	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
log10ws	0.54		Crippen Method
logp	0.017		Crippen Method
mcvol	22.600	ml/mol	McGowan Method
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	22000.00 ± 2000.00	kPa	NIST Webbook
tb	383.76	K	Joback Method
tc	728.00 ± 15.00	K	NIST Webbook
tf	272.26 ± 0.30	K	NIST Webbook
vc	0.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	42.94	J/mol×K	544.30	Joback Method
cpg	41.88	J/mol×K	517.55	Joback Method
cpg	40.79	J/mol×K	490.79	Joback Method
cpg	39.66	J/mol×K	464.03	Joback Method
cpg	38.49	J/mol×K	437.27	Joback Method
cpg	37.29	J/mol×K	410.52	Joback Method
cpg	36.05	J/mol×K	383.76	Joback Method
dvisc	0.9491944	Pa×s	211.40	Joback Method
dvisc	0.0003293	Pa×s	383.76	Joback Method
dvisc	0.0007260	Pa×s	355.03	Joback Method
dvisc	0.0018397	Pa×s	326.31	Joback Method
dvisc	0.0055784	Pa×s	297.58	Joback Method
dvisc	0.0214396	Pa×s	268.85	Joback Method
dvisc	0.1137159	Pa×s	240.13	Joback Method
hvapt	48.50	kJ/mol	320.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65781e+01
Coeff. B	-4.50888e+03
Coeff. C	-4.63500e+01
Temperature range (K), min.	272.74
Temperature range (K), max.	730.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.92300e+02
Coeff. B	-1.71883e+04
Coeff. C	-4.20336e+01
Coeff. D	3.84603e-05

Temperature range (K), min.	288.15
Temperature range (K), max.	390.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1915.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1915
Solubility and Phase Diagram for the Ternary Sodium Oxalate + Hydrogen Peroxide + Water System at (283.15 and 298.15) K:	https://www.doi.org/10.1021/je060461l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7722841&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume