Propiolactone

Other names:	1,3-Propiolactone
	2-Oxacyclobutanone
	2-Oxetanone
	2-Oxooxetane
	3-Hydroxypropionic acid «beta»-lactone
	3-Hydroxypropionic acid Â«betaÂ»-lactone
	3-Hydroxypropionic acid, lactone
	3-Propanolide
	3-Propiolactone
	BPL
	Beta-propiolactone
	Betaprone
	Hydracrylic acid «beta»-lactone
	Hydracrylic acid Â«betaÂ»-lactone
	NSC-21626
	Oxetan-2-one
	Propanoic acid, 3-hydroxy-, «beta»-lactone
	Propanoic acid, 3-hydroxy-, Â«betaÂ»-lactone
	Propanolide
	Propiolactone «beta»-
	Propiolactone Â«betaÂ»-
	Propionic acid, 3-hydroxy-, «beta»-lactone
	Propionic acid, 3-hydroxy-, Â«betaÂ»-lactone
	Propionolactone
	«beta»-Propanoic acid lactone
	«beta»-Propiolactone
	«beta»-Propiolakton
	«beta»-Propionolactone
	«beta»-Propriolactone
	«beta»-Proprolactone
	«beta»-lactone hydracrylic acid
	Â«betaÂ»-Propanoic acid lactone
	Â«betaÂ»-Propiolactone
	Â«betaÂ»-Propiolakton
	Â«betaÂ»-Propionolactone
	Â«betaÂ»-Propriolactone
	Â«betaÂ»-Proprolactone
	Â«betaÂ»-lactone hydracrylic acid
Inchi:	InChI=1S/C3H4O2/c4-3-1-2-5-3/h1-2H2
InchiKey:	VEZXCJBBBCKRPI-UHFFFAOYSA-N

Formula: C3H4O2
SMILES: O=C1CCO1
Mol. weight [g/mol]: 72.06
CAS: 57-57-8

Physical Properties

Property code	Value	Unit	Source
chl	-1419.00 ± 1.20	kJ/mol	NIST Webbook
chl	-1422.30 ± 0.84	kJ/mol	NIST Webbook
gf	-177.97	kJ/mol	Joback Method
hf	-286.20	kJ/mol	NIST Webbook
hf	-282.90	kJ/mol	NIST Webbook
hf	-282.90 ± 0.84	kJ/mol	NIST Webbook
hfl	-329.90 ± 0.84	kJ/mol	NIST Webbook
hfl	-329.90 ± 0.80	kJ/mol	NIST Webbook
hfl	-333.20 ± 1.20	kJ/mol	NIST Webbook
hfus	5.98	kJ/mol	Joback Method
hvap	47.00	kJ/mol	NIST Webbook
hvap	47.03 ± 0.04	kJ/mol	NIST Webbook
hvap	47.00 ± 0.10	kJ/mol	NIST Webbook
ie	9.70 ± 0.01	eV	NIST Webbook
log10ws	0.16		Crippen Method
logp	-0.067		Crippen Method
mcvol	49.710	ml/mol	McGowan Method
pc	5990.66	kPa	Joback Method
sl	175.40	J/mol×K	NIST Webbook
sl	175.30	J/mol×K	NIST Webbook
tb	435.20	K	NIST Webbook
tc	594.39	K	Joback Method
tf	237.02	K	Joback Method
tt	239.86 ± 0.01	K	NIST Webbook
tt	239.86 ± 0.02	K	NIST Webbook
vc	0.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	98.70	J/mol×K	450.46	Joback Method
cpg	91.87	J/mol×K	414.47	Joback Method
cpg	123.16	J/mol×K	594.39	Joback Method
cpg	117.47	J/mol×K	558.40	Joback Method
cpg	111.50	J/mol×K	522.42	Joback Method
cpg	105.24	J/mol×K	486.44	Joback Method
cpg	84.76	J/mol×K	378.49	Joback Method
cpl	122.10	J/mol×K	298.15	NIST Webbook
cpl	122.20	J/mol×K	298.15	NIST Webbook
hfust	9.41	kJ/mol	239.90	NIST Webbook
hfust	9.41	kJ/mol	239.86	NIST Webbook
hfust	9.41	kJ/mol	239.86	NIST Webbook
hvapt	46.40	kJ/mol	379.50	NIST Webbook
sfust	39.23	J/mol×K	239.86	NIST Webbook
sfust	39.23	J/mol×K	239.86	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37466e+01
Coeff. B	-3.63658e+03
Coeff. C	-5.48150e+01
Temperature range (K), min.	325.01
Temperature range (K), max.	485.94

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57578&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume