1,4,7,10,13,16-Hexaoxacyclooctadecane

Other names:	18-crown-6
	18-crown-6 ether
	18-crown-6- ether
	Crown ether 18-crown-6
	ethylene oxide cyclic hexamer
Inchi:	InChI=1S/C12H24O6/c1-2-14-5-6-16-9-10-18-12-11-17-8-7-15-4-3-13-1/h1-12H2
InchiKey:	XEZNGIUYQVAUSS-UHFFFAOYSA-N
Formula:	C12H24O6
SMILES:	C1COCCOCCOCCOCCOCCO1
Mol. weight [g/mol]:	264.32
CAS:	17455-13-9

Physical Properties

Property code	Value	Unit	Source
affp	967.00	kJ/mol	NIST Webbook
basg	909.50	kJ/mol	NIST Webbook
chl	-7061.80 ± 7.50	kJ/mol	NIST Webbook
chs	-7071.00 ± 4.90	kJ/mol	NIST Webbook
gf	-579.60	kJ/mol	Joback Method
hf	-1082.27	kJ/mol	Joback Method
hfs	-1081.10 ± 2.80	kJ/mol	NIST Webbook
hfus	35.50	kJ/mol	The Water 18-Crown-6 System: Experimental Investigation and Thermodynamic Modeling
hsub	119.10 ± 6.70	kJ/mol	NIST Webbook
hvap	86.10 ± 6.70	kJ/mol	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	0.74		Crippen Method
logp	0.100		Crippen Method
mcvol	204.300	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
ripol	2504.00		NIST Webbook
ripol	2504.00		NIST Webbook
tb	711.12	K	Joback Method
tc	981.43	K	Joback Method

tf	312.32	K	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
tf	316.50	K	Static Dielectric Permittivity of Homologous Series of Liquid Cyclic Ethers, 3n-Crown-n, n = 4 to 6
tf	310.00 ± 1.00	K	NIST Webbook
tf	312.25	K	Structure and properties of congruent melting 18-crown-6 crystalline hydrates
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.05	J/mol×K	711.12	Joback Method
cpg	663.41	J/mol×K	756.17	Joback Method
cpg	687.05	J/mol×K	801.22	Joback Method
cpg	707.82	J/mol×K	846.28	Joback Method
cpg	725.59	J/mol×K	891.33	Joback Method
cpg	740.23	J/mol×K	936.38	Joback Method
cpg	751.60	J/mol×K	981.43	Joback Method
dvisc	0.0089867	Pa×s	353.80	Joback Method
dvisc	0.0008700	Pa×s	413.35	Joback Method
dvisc	0.0001517	Pa×s	472.91	Joback Method
dvisc	0.0000391	Pa×s	532.46	Joback Method
dvisc	0.0000132	Pa×s	592.01	Joback Method
dvisc	0.0000055	Pa×s	651.57	Joback Method
dvisc	0.0000026	Pa×s	711.12	Joback Method
hfust	34.00	kJ/mol	312.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.50 ± 0.50	K	0.01	NIST Webbook

tfp	311.76	K	101.30	(Solid + liquid) phase equilibria of binary mixtures containing N-methyl-2-pyrrolidinone and ethers at atmospheric pressure

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Static Dielectric Permittivity of Homologous Series of Liquid Cyclic Ethers, 3n-Crown-n, n = 4 to 6:	https://www.doi.org/10.1021/je300234g
The Water 18-Crown-6 System: Experimental Investigation and Thermodynamic Modeling:	https://www.doi.org/10.1021/je301087w
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemical behavior of 18-crown-6 in aqueous solutions of some monosaccharides:	https://www.doi.org/10.1016/j.tca.2006.02.011
Thermodynamics of complexation of aqueous 18-crown-6 with potassium ion: apparent molar volumes and apparent molar heat capacities of [illegible]	https://www.doi.org/10.1016/j.jct.2004.07.027
Thermodynamics of complexation of aqueous 18-crown-6 with rubidium and [illegible]	https://www.doi.org/10.1016/j.jct.2005.05.005
Thermodynamics of complexation of aqueous 18-crown-6 with barium ion: [illegible]	https://www.doi.org/10.1016/j.jct.2005.01.001
Enthalpies of fusion, vaporization and sublimation of crown ethers [illegible]	https://www.doi.org/10.1016/j.tca.2016.03.013
[illegible]	https://www.doi.org/10.1016/j.jct.2005.01.011
[illegible]	https://www.doi.org/10.1016/j.tca.2005.05.002
[illegible] (18-crown-6 + sodium chloride) at temperatures (278.15 to 393.15) K, at molalities (0.02 to 0.30) mol*kg-1, and at the pressure 0.35 MPa:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17455139&Units=SI
(Solid + liquid) phase equilibria of binary mixtures containing N-methyl-2-pyrrolidinone and ethers at atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2004.11.006
Structure and properties of congruent melting 18-crown-6 crystalline hydrates:	https://www.doi.org/10.1016/j.tca.2010.07.009
Activity Coefficient Studies in Ternary Aqueous Solutions at 298.15 K: H2O + Γ-Cyclodextrin + Potassium Acetate and H2O + 18-Crown-6 + Hydroquinone Systems:	https://www.doi.org/10.1021/je800307g
Compressibility studies of aqueous and CCl4 solutions of 18-crown-6 at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.04.005
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The experimental study on the influence of crown ethers and glycols on the mutual solubility of lithium bromide in water:	https://www.doi.org/10.1016/j.fluid.2018.11.036

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume