

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:	C1COCCOCCOCOCOCOCO1
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	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
tf	312.32	K	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

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

Compressibility studies of aqueous and CCl₄ solutions of 18-crown-6 at T = 293.15 K: Thermodynamics of complexation of aqueous 18-crown-6 with sodium ion: Equilibrium constants, apparent and sublimation enthalpies of aqueous 18-crown-6, sodium chloride, and sucrose, apparent molar volumes, apparent molar heat capacities, and apparent molal volumes of aqueous 18-crown-6 with complexation and aqueous 18-crown-6 with potassium bromide at the pressure 0.35 MPa:

Apparent molar volumes and apparent molar heat capacities of selective 18-crown-6 and of crown-6 with glucose and galactose (dextrose and glucose) in aqueous solutions: Titration, calorimetry, densimetry, viscometry: Thermodynamics of complexation of aqueous 18-crown-6 with barium ion:

Apparent molar volumes of aqueous 18-crown-6. Systematic experimental investigation of aqueous 18-crown-6 and barium nitrate at temperatures (278.15 to 393.15) K, at molalities (0.02 to 0.33) mol.kg⁻¹, and at influence of crown ethers and glycols on the mutual solubility in ternary aqueous solutions at 298.15 K: H₂O + sucrose + 18-crown-6 phase equilibrium state and binary mixtures containing quinone systems: N,N-dimethylpyrrolidinone and ethers at atmospheric pressure:

Thermodynamics of complexation of aqueous 18-crown-6 with rubidium and cesium ions: Apparent molar volumes 18-crown-6 molalities, equilibrium constants, and properties of congruent melting 18-crown-6·crystalline rubidium chloride and 18-crown-6·cesium chloride at temperatures (278.15 to 393.15) K, at molalities (0.02 to 0.33) mol.kg⁻¹, and at the pressure 0.35 MPa:

- <https://www.doi.org/10.1016/j.jct.2005.04.005>
- <https://www.doi.org/10.1016/j.jct.2005.01.011>
- <https://www.doi.org/10.1016/j.tca.2016.03.013>
- <https://www.doi.org/10.1021/je300234g>
- <https://www.doi.org/10.1016/j.jct.2004.07.027>
- https://www.chemeo.com/doc/models/crippen_log10ws
- <https://www.doi.org/10.1016/j.tca.2005.05.002>
- <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
- <https://www.doi.org/10.1016/j.jct.2005.01.001>
- <https://www.doi.org/10.1021/je301087w>
- https://en.wikipedia.org/wiki/Joback_method
- <https://www.doi.org/10.1016/j.fluid.2018.11.036>
- <https://www.doi.org/10.1021/je800307g>
- <https://www.doi.org/10.1016/j.fluid.2004.11.006>
- <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17455139&Units=SI>
- <https://www.doi.org/10.1016/j.jct.2005.05.005>
- <https://www.doi.org/10.1016/j.tca.2006.02.011>
- <https://www.doi.org/10.1016/j.tca.2010.07.009>
- <http://link.springer.com/article/10.1007/BF02311772>

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
mvol:	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

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