12-Crown-4

Other names:	1,4,7,10-tetraoxacyclododecane
	12-crown-4 ether
	Eoct
	Ethylene oxide cyclic tetramer
Inchi:	InChI=1S/C8H16O4/c1-2-10-5-6-12-8-7-11-4-3-9-1/h1-8H2
InchiKey:	XQQZRZQVBFHBHL-UHFFFAOYSA-N
Formula:	C8H16O4
SMILES:	C1COCCOCCOCCO1
Mol. weight [g/mol]:	176.21
CAS:	294-93-9

Physical Properties

Property code	Value	Unit	Source
affp	927.20	kJ/mol	NIST Webbook
basg	890.50	kJ/mol	NIST Webbook
chl	-4738.10 ± 1.70	kJ/mol	NIST Webbook
gf	-368.44	kJ/mol	Joback Method
hf	-631.10 ± 2.10	kJ/mol	NIST Webbook
hfl	-696.80 ± 2.10	kJ/mol	NIST Webbook
hfus	26.56	kJ/mol	Joback Method
hvap	65.65 ± 0.37	kJ/mol	NIST Webbook
hvap	65.60 ± 0.40	kJ/mol	NIST Webbook
hvap	65.70	kJ/mol	NIST Webbook
hvap	65.70 ± 3.70	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	0.58		Crippen Method
logp	0.066		Crippen Method
mcvol	136.200	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	540.08	K	Joback Method
tc	788.65	K	Joback Method
tf	289.00	K	Static Dielectric Permittivity of Homologous Series of Liquid Cyclic Ethers, 3n-Crown-n, n = 4 to 6

vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.89	J/mol×K	540.08	Joback Method
cpg	362.26	J/mol×K	581.51	Joback Method
cpg	382.34	J/mol×K	622.94	Joback Method
cpg	401.09	J/mol×K	664.36	Joback Method
cpg	418.48	J/mol×K	705.79	Joback Method
cpg	434.46	J/mol×K	747.22	Joback Method
cpg	449.00	J/mol×K	788.65	Joback Method
dvisc	0.0436594	Pa×s	276.70	Joback Method
dvisc	0.0072676	Pa×s	320.60	Joback Method
dvisc	0.0018632	Pa×s	364.49	Joback Method
dvisc	0.0006401	Pa×s	408.39	Joback Method
dvisc	0.0002705	Pa×s	452.29	Joback Method
dvisc	0.0001332	Pa×s	496.18	Joback Method
dvisc	0.0000736	Pa×s	540.08	Joback Method
hfust	22.46	kJ/mol	290.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C294939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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-water:	https://www.doi.org/10.1016/j.fluid.2018.11.036
Static Dielectric Permittivity of Homologous Series of Liquid Cyclic Ethers, 5H-Crown-n, n = 4 to 6:	https://www.doi.org/10.1021/je300234g
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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