15-Crown-5

Other names: 1,4,10,13-pentaoxacyclopentadecane
1,4,7,10,13-pentaoxacyclopentadecane
15-crown-5 ether
Inchi: InChI=1S/C10H20O5/c1-2-12-5-6-14-9-10-15-8-7-13-4-3-11-1/h1-10H2
InchiKey: VFTFKUDGYRBSAL-UHFFFAOYSA-N
Formula: C10H20O5
SMILES: C1COCCOCCOCCOCCO1
Mol. weight [g/mol]: 220.26
CAS: 33100-27-5

Physical Properties

Property code	Value	Unit	Source
affp	943.80	kJ/mol	NIST Webbook
basg	899.70	kJ/mol	NIST Webbook
chl	-5903.00 ± 7.30	kJ/mol	NIST Webbook
chl	-5914.30 ± 1.40	kJ/mol	NIST Webbook
gf	-474.02	kJ/mol	Joback Method
hf	-799.50 ± 2.00	kJ/mol	NIST Webbook
hfl	-879.10 ± 2.00	kJ/mol	NIST Webbook
hfus	33.41	kJ/mol	Joback Method
hvap	75.70 ± 1.70	kJ/mol	NIST Webbook
hvap	79.60 ± 0.30	kJ/mol	NIST Webbook
hvap	79.60	kJ/mol	NIST Webbook
hvap	79.57	kJ/mol	NIST Webbook
hvap	79.57 ± 0.29	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.58	eV	NIST Webbook
log10ws	0.66		Crippen Method
logp	0.083		Crippen Method
mcvol	170.250	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1554.00		NIST Webbook
ripol	2431.00		NIST Webbook
tb	625.60	K	Joback Method
tc	886.64	K	Joback Method

tf	253.00	K	Static Dielectric Permittivity of Homologous Series of Liquid Cyclic Ethers, 3n-Crown-n, n = 4 to 6
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.77	J/mol×K	625.60	Joback Method
cpg	506.63	J/mol×K	669.11	Joback Method
cpg	529.59	J/mol×K	712.61	Joback Method
cpg	550.55	J/mol×K	756.12	Joback Method
cpg	569.43	J/mol×K	799.63	Joback Method
cpg	586.16	J/mol×K	843.13	Joback Method
cpg	600.65	J/mol×K	886.64	Joback Method
dvisc	0.0244532	Pa×s	315.25	Joback Method
dvisc	0.0030189	Pa×s	366.98	Joback Method
dvisc	0.0006249	Pa×s	418.70	Joback Method
dvisc	0.0001829	Pa×s	470.43	Joback Method
dvisc	0.0000683	Pa×s	522.15	Joback Method
dvisc	0.0000305	Pa×s	573.88	Joback Method
dvisc	0.0000155	Pa×s	625.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	0.03	NIST Webbook
tbrp	351.00	K	0.01	NIST Webbook

Sources

Measurements of binary diffusion coefficients and retention factors for dibenzo-24-crown-8 and 15-crown-5 in supercritical carbon dioxide by chromatographic impulse response technique: https://www.doi.org/10.1016/j.fluid.2007.01.035

The experimental study on the influence of crown ethers and glycols on the dielectric permittivity of water: https://www.doi.org/10.1016/j.fluid.2018.11.036

Static Dielectric Permittivity of Homologous Series of Liquid Cyclic Ethers, 3n-Crown-n, n = 4 to 6: https://www.doi.org/10.1021/je300234g

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=C33100275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume