1,4,7,10,13-Benzopentaoxacyclopentadecin, 2,3,5,6,8,9,11,12-octahydro-

Other names: Benzo[6]1,4,7,10,13-pentaoxacyclopentadecane
Benzo-15-crown-5
Benzo-15-crown-5 ether
Crown ether benzo-15-crown-5
Monobenzo-15-crown-5
2,3-Benzo-15-crown-5
2,3,5,6,8,9,11,12-Octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin
Bis(1,4,7,10,13-benzopentaoxacyclopentadecin, 2,3,5,6,8,9,11,12-octahydro-)

Inchi: InChI=1S/C14H20O5/c1-2-4-14-13(3-1)18-11-9-16-7-5-15-6-8-17-10-12-19-14/h1-4H,5-1

InchiKey: FNEPSTUXZLEUCK-UHFFFAOYSA-N

Formula: C14H20O5

SMILES: c1ccc2c(c1)OCCOCCOCCOCCO2

Mol. weight [g/mol]: 268.31

CAS: 14098-44-3

Physical Properties

Property code	Value	Unit	Source
chs	-7585.10 ± 6.20	kJ/mol	NIST Webbook
gf	-313.36	kJ/mol	Joback Method
hf	-735.69	kJ/mol	Joback Method
hfs	-782.40 ± 4.70	kJ/mol	NIST Webbook
hfus	41.63	kJ/mol	Joback Method
hsub	128.00 ± 11.00	kJ/mol	NIST Webbook
hvap	98.90 ± 1.30	kJ/mol	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-1.38		Crippen Method
logp	1.508		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	740.24	K	Joback Method
tc	1011.97	K	Joback Method
tf	354.10 ± 0.30	K	NIST Webbook
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.55	J/mol×K	740.24	Joback Method
cpg	638.34	J/mol×K	785.53	Joback Method
cpg	657.74	J/mol×K	830.82	Joback Method
cpg	674.72	J/mol×K	876.11	Joback Method
cpg	689.24	J/mol×K	921.39	Joback Method
cpg	701.27	J/mol×K	966.68	Joback Method
cpg	710.78	J/mol×K	1011.97	Joback Method
dvisc	0.0016698	Pa×s	406.31	Joback Method
dvisc	0.0004255	Pa×s	461.97	Joback Method
dvisc	0.0001455	Pa×s	517.62	Joback Method
dvisc	0.0000613	Pa×s	573.27	Joback Method
dvisc	0.0000301	Pa×s	628.93	Joback Method
dvisc	0.0000166	Pa×s	684.59	Joback Method
dvisc	0.0000100	Pa×s	740.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14098443&Units=SI

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

Legend

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume