1,4,7,10-Benzotetraoxacyclododecin, 2,3,5,6,8,9-hexahydro-

Other names: Benzo-12-crown 4-ether
Benzo-12-crown-4
2,3-Benzo-1,4,7,10-tetraoxacyclododecane

Inchi: InChI=1S/C12H16O4/c1-2-4-12-11(3-1)15-9-7-13-5-6-14-8-10-16-12/h1-4H,5-10H2

InchiKey: OAJNZFCPJVBYHB-UHFFFAOYSA-N

Formula: C12H16O4

SMILES: c1ccc2c(c1)OCCOCCOCCO2

Mol. weight [g/mol]: 224.25

CAS: 14174-08-4

Physical Properties

Property code	Value	Unit	Source
gf	-207.78	kJ/mol	Joback Method
hf	-543.93	kJ/mol	Joback Method
hfus	34.77	kJ/mol	Joback Method
hsub	104.30 ± 2.60	kJ/mol	NIST Webbook
hvap	82.70 ± 2.30	kJ/mol	NIST Webbook
log10ws	-1.45		Crippen Method
logp	1.491		Crippen Method
mcvol	168.800	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	654.72	K	Joback Method
tc	918.02	K	Joback Method
tf	367.76	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.22	J/mol×K	654.72	Joback Method
cpg	487.59	J/mol×K	698.60	Joback Method
cpg	506.20	J/mol×K	742.49	Joback Method
cpg	523.06	J/mol×K	786.37	Joback Method
cpg	538.19	J/mol×K	830.25	Joback Method

cpg	551.58	J/mol×K	874.14	Joback Method
cpg	563.26	J/mol×K	918.02	Joback Method
dvisc	0.0033280	Pa×s	367.76	Joback Method
dvisc	0.0010939	Pa×s	415.59	Joback Method
dvisc	0.0004524	Pa×s	463.41	Joback Method
dvisc	0.0002207	Pa×s	511.24	Joback Method
dvisc	0.0001217	Pa×s	559.07	Joback Method
dvisc	0.0000738	Pa×s	606.89	Joback Method
dvisc	0.0000481	Pa×s	654.72	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14174084&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: 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
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