DIBENZO-18-CROWN-6

Other names: 2,3:11,12-dibenzo-1,4,7,10,13,16-hexaoxacyclooctadecane
6,7,9,10,17,18,20,21-octahydrodibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin
Crown ether dibenzo-18-crown-6
Dibenzo-18-crown-6-ether
Dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin, 6,7,9,10,17,18,20,21-octahydro-
NSC 147771
crown 18
crown-18
dibenzo[a,j]-1,4,7,10,13,16-hexaoxacyclooctadeca-2,11-diene
dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecane
dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin, 6,7,9,10,17,18,20,21-octahydro-

Inchi: InChI=1S/C20H24O6/c1-2-6-18-17(5-1)23-13-9-21-11-15-25-19-7-3-4-8-20(19)26-16-12-

InchiKey: YSSSPARMOAYJTE-UHFFFAOYSA-N

Formula: C20H24O6

SMILES: c1ccc2c(c1)OCCOCCOc1ccccc1OCCOCCO2

Mol. weight [g/mol]: 360.41

Physical Properties

Property code	Value	Unit	Source
chs	-10477.80 ± 4.80	kJ/mol	NIST Webbook
hf	-671.62	kJ/mol	Cheméo Relay (1.0)
hfs	-822.40 ± 2.40	kJ/mol	NIST Webbook
hfus	55.95	kJ/mol	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
hsub	178.80 ± 6.90	kJ/mol	NIST Webbook
hvap	137.00 ± 7.40	kJ/mol	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
log10ws	-3.88		Cheméo Relay (1.0)
logp	2.949		Crippen Method
mcvol	269.500	ml/mol	McGowan Method
tb	751.36	K	Cheméo Relay (1.0)
tf	434.00 ± 1.00	K	NIST Webbook

tf	435.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.91	J/mol×K	940.40	Joback Method
cpg	914.55	J/mol×K	987.74	Joback Method
cpg	925.82	J/mol×K	1035.09	Joback Method
cpg	933.72	J/mol×K	1082.43	Joback Method
cpg	938.22	J/mol×K	1129.78	Joback Method
cpg	939.31	J/mol×K	1177.12	Joback Method
cpg	936.98	J/mol×K	1224.46	Joback Method
dvisc	0.0001312	Pa×s	535.92	Joback Method
dvisc	0.0000408	Pa×s	603.33	Joback Method
dvisc	0.0000161	Pa×s	670.75	Joback Method
dvisc	0.0000075	Pa×s	738.16	Joback Method
dvisc	0.0000040	Pa×s	805.57	Joback Method
dvisc	0.0000023	Pa×s	872.99	Joback Method
dvisc	0.0000015	Pa×s	940.40	Joback Method
hfust	57.45	kJ/mol	435.80	NIST Webbook
hfust	57.46	kJ/mol	435.75	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry: https://www.doi.org/10.1016/j.tca.2016.03.013

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14187327&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point