DIBENZO-24-CROWN-8

Other names: 2,3,14,15-Dibenzo-1,4,7,10,13,16,19,22-octaoxacyclotetracosa-2,14-diene
6,7,9,10,12,13,20,21,23,24,26,27-dodecahydrodibenz[b,n][1,4,7,10,13,16,19,22]octaoxac
Crown ether dibenzo-24-crown-8
Dibenzo-24-crown 8-ether
dibenz[b,n][1,4,7,10,13,16,19,22]octaoxacyclotetracosin, 6,7,9,10,12,13,20,21,23,24,26,27-dodecahydro-
«beta»-Dibenzo-24-crown-8

Inchi: InChI=1S/C24H32O8/c1-2-6-22-21(5-1)29-17-13-25-9-10-27-15-19-31-23-7-3-4-8-24(23)
InchiKey: UNTITLLXXOKDTB-UHFFFAOYSA-N
Formula: C24H32O8
SMILES: c1ccc2c(c1)OCCOCCOCCOc1ccccc1OCCOCCOCCO2
Mol. weight [g/mol]: 448.51

Physical Properties

Property code	Value	Unit	Source
hf	-1006.13	kJ/mol	Cheméo Relay (1.0)
hfus	70.42	kJ/mol	Joback Method
hvap	151.10	kJ/mol	Cheméo Relay (1.0)
ie	7.48	eV	Cheméo Relay (1.0)
log10ws	-3.76		Cheméo Relay (1.0)
logp	2.982		Crippen Method
mcvol	337.600	ml/mol	McGowan Method
tb	825.77	K	Cheméo Relay (1.0)
tf	373.87	K	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
tf	381.41 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.43	J/mol×K	1111.44	Joback Method
cpg	1192.92	J/mol×K	1160.45	Joback Method

cpg	1186.68	J/mol×K	1209.45	Joback Method
cpg	1174.58	J/mol×K	1258.46	Joback Method
cpg	1156.50	J/mol×K	1307.47	Joback Method
cpg	1132.31	J/mol×K	1356.48	Joback Method
cpg	1101.89	J/mol×K	1405.48	Joback Method
dvisc	0.0000084	Pa×s	613.02	Joback Method
dvisc	0.0000019	Pa×s	696.09	Joback Method
dvisc	0.0000006	Pa×s	779.16	Joback Method
dvisc	0.0000002	Pa×s	862.23	Joback Method
dvisc	0.0000001	Pa×s	945.30	Joback Method
dvisc	5.2208154e-08	Pa×s	1028.37	Joback Method
dvisc	2.9814006e-08	Pa×s	1111.44	Joback Method
hfust	52.25	kJ/mol	375.40	NIST Webbook
hfust	15.45	kJ/mol	234.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14174095&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
Cheméo Relay (1.0):	
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point