

dibenzo-30-crown-10

Other names:	6,7,9,10,12,13,15,16,23,24,26,27,29,30,32,33-hexadecahydrodibenzo[b,q][1,4,7,10,13,16]octaphthalene
Inchi:	InChI=1S/C28H40O10/c1-2-6-26-25(5-1)35-21-17-31-13-9-29-11-15-33-19-23-37-27-7-3
InchiKey:	MXCSCGRLMRZMF-UHFFFAOYSA-N
Formula:	C28H40O10
SMILES:	<chem>c1ccc2c(c1)OCCOCCOCCOCCOc1ccccc1OCCOCCOCCOCCO2</chem>
Mol. weight [g/mol]:	536.62

Physical Properties

Property code	Value	Unit	Source
gf	-680.60	kJ/mol	Joback Method
hf	-1539.67	kJ/mol	Joback Method
hfus	86.53	kJ/mol	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
hvap	133.08	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.015		Crippen Method
mcvol	405.700	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
tb	1282.48	K	Joback Method
tc	1590.25	K	Joback Method
tf	377.60	K	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.70	J/molxK	1538.96	Joback Method

cpg	1370.17	J/mol×K	1333.78	Joback Method
cpg	1327.37	J/mol×K	1385.07	Joback Method
cpg	1274.86	J/mol×K	1436.37	Joback Method
cpg	1212.39	J/mol×K	1487.66	Joback Method
cpg	1403.54	J/mol×K	1282.48	Joback Method
cpg	1056.51	J/mol×K	1590.25	Joback Method
cpl	1187.90	J/mol×K	430.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1148.90	J/mol×K	395.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1153.00	J/mol×K	400.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1159.50	J/mol×K	405.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1164.60	J/mol×K	410.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

cpl	1169.30	J/molxK	415.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1179.20	J/molxK	420.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1144.60	J/molxK	390.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1202.00	J/molxK	465.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1201.60	J/molxK	460.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1200.90	J/molxK	455.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

cpl	1201.20	J/molxK	450.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1201.90	J/molxK	470.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1196.60	J/molxK	440.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1195.00	J/molxK	435.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1199.20	J/molxK	445.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cpl	1186.20	J/molxK	425.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

cps	755.50	J/mol×K	325.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	826.40	J/mol×K	350.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	811.50	J/mol×K	345.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	797.00	J/mol×K	340.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	783.30	J/mol×K	335.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	769.90	J/mol×K	330.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

cps	844.90	J/mol×K	355.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	741.60	J/mol×K	320.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	728.40	J/mol×K	315.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	715.30	J/mol×K	310.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	700.30	J/mol×K	305.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	686.90	J/mol×K	300.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

cps	680.40	J/molxK	298.15	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	868.20	J/molxK	360.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
cps	668.80	J/molxK	295.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
dvisc	4.4800360e-10	Paxs	1282.48	Joback Method
dvisc	0.0000003	Paxs	690.12	Joback Method
dvisc	5.3958678e-08	Paxs	788.85	Joback Method
dvisc	1.3512811e-08	Paxs	887.57	Joback Method
dvisc	4.4648933e-09	Paxs	986.30	Joback Method
dvisc	1.8046668e-09	Paxs	1085.03	Joback Method
dvisc	8.4840951e-10	Paxs	1183.75	Joback Method
pvap	0.10	kPa	570.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.06	kPa	560.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.08	kPa	565.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.09	kPa	570.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.12	kPa	575.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.15	kPa	580.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.18	kPa	585.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.21	kPa	590.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.27	kPa	595.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.08	kPa	565.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.07	kPa	560.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.05	kPa	555.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.04	kPa	550.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.03	kPa	545.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.27	kPa	595.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.22	kPa	590.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.19	kPa	585.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.14	kPa	580.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.12	kPa	575.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.09	kPa	570.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.08	kPa	565.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.06	kPa	560.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.05	kPa	555.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.04	kPa	550.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.03	kPa	545.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.05	kPa	555.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.04	kPa	550.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.04	kPa	545.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.26	kPa	595.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.22	kPa	590.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.18	kPa	585.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.14	kPa	580.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.12	kPa	575.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
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Sources

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
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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase 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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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