Coronene

Other names:	Dibenzo(ghi,pqr)perylene
	Hexabenzobenzene
	dibenzo[ghi,pqr]perylene
Inchi:	InChI=1S/C24H12/c1-2-14-5-6-16-9-11-18-12-10-17-8-7-15-4-3-13(1)19-20(14)22(16)24(
InchiKey:	VPUGDVKSAQVFFS-UHFFFAOYSA-N
Formula:	C24H12
SMILES:	c1cc2ccc3ccc4ccc5ccc6ccc1c1c2c3c4c5c61
Mol. weight [g/mol]:	300.35
CAS:	191-07-1

Physical Properties

Property code	Value	Unit	Source
affp	861.30	kJ/mol	NIST Webbook
affp	859.40	kJ/mol	NIST Webbook
basg	836.80	kJ/mol	NIST Webbook
basg	835.00	kJ/mol	NIST Webbook
ea	0.47 ± 0.09	eV	NIST Webbook
ea	0.54 ± 0.10	eV	NIST Webbook
gf	838.08	kJ/mol	Joback Method
hf	295.00 ± 11.00	kJ/mol	NIST Webbook
hfs	152.30 ± 6.90	kJ/mol	NIST Webbook
hfus	21.20	kJ/mol	The thermochemistry of coronene revisited
hsub	131.00 ± 1.70	kJ/mol	NIST Webbook
hsub	142.60 ± 8.70	kJ/mol	NIST Webbook
hsub	128.00	kJ/mol	NIST Webbook
hvap	148.00 ± 0.50	kJ/mol	NIST Webbook
ie	7.68 ± 0.05	eV	NIST Webbook
ie	7.34	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	7.29 ± 0.03	eV	NIST Webbook
ie	7.29	eV	NIST Webbook
ie	7.29	eV	NIST Webbook
ie	7.44	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	7.65	eV	NIST Webbook

ie	7.64	eV	NIST Webbook
ie	7.70 ± 0.10	eV	NIST Webbook
ie	7.26 ± 0.05	eV	NIST Webbook
ie	7.29	eV	NIST Webbook
log10ws	-9.33		Estimated Solubility Method
log10ws	-9.33		Aqueous Solubility Prediction Method
logp	6.919		Crippen Method
mcvol	221.400	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	3498.00		NIST Webbook
rinpol	549.07		NIST Webbook
rinpol	549.65		NIST Webbook
rinpol	550.43		NIST Webbook
rinpol	549.07		NIST Webbook
rinpol	550.43		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	548.36		NIST Webbook
rinpol	549.10		NIST Webbook
rinpol	593.50		NIST Webbook
rinpol	534.99		NIST Webbook
rinpol	551.76		NIST Webbook
rinpol	591.61		NIST Webbook
rinpol	554.42		NIST Webbook
rinpol	574.73		NIST Webbook
rinpol	529.07		NIST Webbook
rinpol	3498.00		NIST Webbook
rinpol	3456.00		NIST Webbook
rinpol	3497.00		NIST Webbook
rinpol	3498.00		NIST Webbook
rinpol	3498.00		NIST Webbook
rinpol	554.42		NIST Webbook
rinpol	3497.00		NIST Webbook
ss	280.90	J/mol×K	NIST Webbook
tb	798.20	K	NIST Webbook
tc	1154.51	K	Joback Method
tf	710.50 ± 0.20	K	NIST Webbook
tf	688.15 ± 2.50	K	NIST Webbook
tf	711.58	K	Aqueous Solubility Prediction Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.52	J/mol×K	890.88	Joback Method
cpg	639.68	J/mol×K	934.82	Joback Method
cpg	654.66	J/mol×K	978.76	Joback Method
cpg	670.86	J/mol×K	1022.70	Joback Method
cpg	688.72	J/mol×K	1066.64	Joback Method
cpg	708.65	J/mol×K	1110.57	Joback Method
cpg	731.08	J/mol×K	1154.51	Joback Method
cps	313.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0266312	Pa×s	664.30	Joback Method
dvisc	0.0275768	Pa×s	702.06	Joback Method
dvisc	0.0284544	Pa×s	739.83	Joback Method
dvisc	0.0292708	Pa×s	777.59	Joback Method
dvisc	0.0300317	Pa×s	815.35	Joback Method
dvisc	0.0314079	Pa×s	890.88	Joback Method
dvisc	0.0307426	Pa×s	853.12	Joback Method
hfust	21.20	kJ/mol	709.00	NIST Webbook
hfust	19.20	kJ/mol	710.50	NIST Webbook
hfust	19.20	kJ/mol	710.50	NIST Webbook
hsubt	126.60 ± 1.70	kJ/mol	478.00	NIST Webbook
hsubt	133.10 ± 5.10	kJ/mol	462.50	NIST Webbook
hsubt	143.20	kJ/mol	383.00	NIST Webbook
hsubt	135.90	kJ/mol	468.50	NIST Webbook
hsubt	147.00	kJ/mol	473.00	NIST Webbook
hsubt	143.20	kJ/mol	515.50	NIST Webbook
hsubt	148.50	kJ/mol	407.00	NIST Webbook
hvapt	104.20	kJ/mol	398.00	NIST Webbook

Sources

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C191071&Units=SI

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

The thermochemistry of coronene revisited: https://www.doi.org/10.1016/j.jct.2009.03.010

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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