Hexabenzo[bc:ef:hi:kl:no:qr]coronene

Other names:	1:12,2:3,4:5,6:7,8:9,10:11-Hexabenzocoronene
	Hexabenzo[bc,ef,hi,kl,no,qr]coronene
Inchi:	InChI=1S/C42H18/c1-7-19-21-9-2-11-23-25-13-4-15-27-29-17-6-18-30-28-16-5-14-26-24
InchiKey:	IVJZBYVRLJZOOQ-UHFFFAOYSA-N
Formula:	C42H18
SMILES:	c1cc2c3cccc4c5cccc6c7cccc8c9cccc%10c%11cccc%12c(c1)c2c1c(c34)c(c56)c(c78)c(c%
Mol. weight [g/mol]:	522.59
CAS:	190-24-9

Physical Properties

Property code	Value	Unit	Source
gf	1554.48	kJ/mol	Joback Method
hf	1220.23	kJ/mol	Joback Method
hfus	76.39	kJ/mol	Joback Method
hvap	134.51	kJ/mol	Joback Method
log10ws	-19.62		Crippen Method
logp	12.152		Crippen Method
mcvol	371.160	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
tb	1423.38	K	Joback Method
tc	1742.76	K	Joback Method
tf	1157.32	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1649.96	J/mol×K	1423.38	Joback Method
cpg	1773.63	J/mol×K	1476.61	Joback Method
cpg	1914.44	J/mol×K	1529.84	Joback Method
cpg	2073.78	J/mol×K	1583.07	Joback Method
cpg	2253.07	J/mol×K	1636.30	Joback Method
cpg	2453.70	J/mol×K	1689.53	Joback Method
cpg	2677.06	J/mol×K	1742.76	Joback Method

dvisc	15.4036521	Pa×s	1157.32	Joback Method
dvisc	16.3249731	Pa×s	1201.66	Joback Method
dvisc	17.2300107	Pa×s	1246.01	Joback Method
dvisc	18.1179079	Pa×s	1290.35	Joback Method
dvisc	18.9880560	Pa×s	1334.69	Joback Method
dvisc	19.8400516	Pa×s	1379.04	Joback Method
dvisc	20.6736601	Pa×s	1423.38	Joback Method

Sources

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=C190249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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