1,2,9,10-Dibenzopyrene

Other names:	Dibenzo[def,p]chrysene
	1,2:3,4-Dibenzopyrene
	Ba 51-090462
	Dibenzo[a,l]pyrene
	1,2:9,10-Dibenzopyrene
	4,5:6,7-Dibenzpyrene
	Db(a,l)p
	Dibenzo(a,d)pyrene
	4,5,6,7-Dibenzpyrene
	2,3:4,5-Dibenzopyrene
	Dibenz[a,l]pyrene
	NSC 90324
	Dibenzo(a,1)pyrene
	1,2,4,5-Dibenzpyrene
	1,2,3,4-Dibenzpyrene
	1,2:9,1o-Dibenzopyrene
Inchi:	InChI=1S/C24H14/c1-2-8-18-16(6-1)14-17-13-12-15-7-5-11-20-19-9-3-4-10-21(19)24(18)
InchiKey:	JNTHRSHGARDABO-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	c1ccc2c(c1)cc1ccc3cccc4c5ccccc5c2c1c34
Mol. weight [g/mol]:	302.37
CAS:	191-30-0

Physical Properties

Property code	Value	Unit	Source
gf	752.58	kJ/mol	Joback Method
hf	561.85	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
ie	7.03	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
log10ws	-9.91		Crippen Method
logp	6.890		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	553.00		NIST Webbook
rinpol	541.90		NIST Webbook

rinpol	3423.00		NIST Webbook
rinpol	538.21		NIST Webbook
rinpol	538.21		NIST Webbook
rinpol	3423.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	540.01		NIST Webbook
tb	882.32	K	Joback Method
tc	1151.38	K	Joback Method
tf	501.20 ± 0.40	K	NIST Webbook
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.66	J/mol×K	882.32	Joback Method
cpg	676.44	J/mol×K	927.16	Joback Method
cpg	691.24	J/mol×K	972.01	Joback Method
cpg	706.42	J/mol×K	1016.85	Joback Method
cpg	722.35	J/mol×K	1061.69	Joback Method
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
dvisc	0.0049439	Pa×s	652.49	Joback Method
dvisc	0.0052883	Pa×s	606.52	Joback Method
dvisc	0.0046630	Pa×s	698.45	Joback Method
dvisc	0.0044300	Pa×s	744.42	Joback Method
dvisc	0.0042338	Pa×s	790.39	Joback Method
dvisc	0.0040664	Pa×s	836.35	Joback Method
dvisc	0.0039222	Pa×s	882.32	Joback Method
hfust	24.68	kJ/mol	501.20	NIST Webbook
hfust	24.68	kJ/mol	501.20	NIST Webbook

Sources

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

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

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=C191300&Units=SI

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
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume