1,2:4,5-Dibenzopyrene

Other names:	Naphtho[1,2,3,4-def]chrysene
	Dibenzo[a,e]pyrene
	Db(a,e)P
	1,2,4,5-Dibenzopyrene
	1,2:4,5-Dibenzpyrene
	dibenz[a,e]pyrene
	Naphtho[1,2,3,4-de]chrysene
Inchi:	InChI=1S/C24H14/c1-2-8-17-16(6-1)14-22-19-10-4-3-9-18(19)20-11-5-7-15-12-13-21(17)
InchiKey:	KGHMWBNEMFNJFZ-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	c1ccc2c(c1)cc1c3ccccc3c3cccc4ccc2c1c43
Mol. weight [g/mol]:	302.37
CAS:	192-65-4

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	7.41	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.11	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	551.53		NIST Webbook
rinpol	3507.00		NIST Webbook
rinpol	3540.00		NIST Webbook
rinpol	3507.00		NIST Webbook
rinpol	555.26		NIST Webbook
rinpol	3507.00		NIST Webbook
rinpol	553.40		NIST Webbook
rinpol	554.76		NIST Webbook
rinpol	551.65		NIST Webbook

rinpol	551.53		NIST Webbook
rinpol	551.65		NIST Webbook
rinpol	584.60		NIST Webbook
rinpol	551.53		NIST Webbook
rinpol	554.05		NIST Webbook
rinpol	3540.00		NIST Webbook
rinpol	555.26		NIST Webbook
rinpol	3507.00		NIST Webbook
rinpol	551.65		NIST Webbook
rinpol	554.05		NIST Webbook
tb	882.32	K	Joback Method
tc	1151.38	K	Joback Method
tf	520.20 ± 0.50	K	NIST Webbook
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
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
dvisc	0.0040664	Pa×s	836.35	Joback Method
dvisc	0.0039222	Pa×s	882.32	Joback Method
dvisc	0.0052883	Pa×s	606.52	Joback Method
dvisc	0.0049439	Pa×s	652.49	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
hfust	30.50	kJ/mol	520.20	NIST Webbook
hfust	30.50	kJ/mol	520.20	NIST Webbook
hfust	32.10	kJ/mol	517.90	NIST Webbook
hsubt	137.60	kJ/mol	480.00	NIST Webbook
hsubt	146.40	kJ/mol	460.00	NIST Webbook

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=C192654&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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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

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