Picene

Other names:	1,2,7,8-Dibenzphenanthrene
	1,2:7,8-Dibenzophenanthrene
	1,2:7,8-Dibenzphenanthrene
	3,4-Benzchrysene
	Benzo(a)chrysene
	Dibenzo(a,i)phenanthrene
	NSC 406006
	Pycene
	«beta»,«beta»-Binaphthyleneethene
	Â«betaÂ»,Â«betaÂ»-Binaphthyleneethene
Inchi:	InChI=1S/C22H14/c1-3-7-17-15(5-1)9-11-21-19(17)13-14-20-18-8-4-2-6-16(18)10-12-22(
InchiKey:	GBROPGWFBFCKAG-UHFFFAOYSA-N
Formula:	C22H14
SMILES:	c1ccc2c(c1)ccc1c2ccc2c3ccccc3ccc21
Mol. weight [g/mol]:	278.35
CAS:	213-46-7

Physical Properties

Property code	Value	Unit	Source
affp	851.30	kJ/mol	NIST Webbook
affp	843.50	kJ/mol	NIST Webbook
basg	818.00	kJ/mol	NIST Webbook
basg	820.60	kJ/mol	NIST Webbook
ea	0.54 ± 0.01	eV	NIST Webbook
gf	644.48	kJ/mol	Joback Method
hf	468.99	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
ie	7.54 ± 0.04	eV	NIST Webbook
ie	7.48 ± 0.05	eV	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.62	eV	NIST Webbook
ie	7.52 ± 0.02	eV	NIST Webbook
ie	7.52	eV	NIST Webbook
ie	7.51 ± 0.02	eV	NIST Webbook

ie	7.80 ± 0.10	eV	NIST Webbook
log10ws	-7.87		Estimated Solubility Method
log10ws	-7.87		Aqueous Solubility Prediction Method
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	3213.00		NIST Webbook
rinpol	3159.00		NIST Webbook
rinpol	3140.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3177.00		NIST Webbook
rinpol	3179.00		NIST Webbook
rinpol	3159.00		NIST Webbook
rinpol	3214.00		NIST Webbook
rinpol	3227.00		NIST Webbook
rinpol	3227.00		NIST Webbook
rinpol	3159.00		NIST Webbook
rinpol	3140.00		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	532.48	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	607.64	J/mol×K	820.30	Joback Method
cpg	650.13	J/mol×K	955.09	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method
dvisc	0.0022584	Pa×s	532.48	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method

hfust	35.19	kJ/mol	637.20	NIST Webbook
hfust	35.19	kJ/mol	637.20	NIST Webbook
hsubt	140.10	kJ/mol	456.50	NIST Webbook
hsubt	140.70	kJ/mol	468.00	NIST Webbook

Sources

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=C213467&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
ea: Electron affinity
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