Indeno[1,2,3-cd]pyrene

Other names:	1,10-(1,2-Phenylene)pyrene
	1,10-(o-Phenylene)pyrene
	1,10-(ortho-Phenylene)pyrene
	2,3-(o-Phenylene)pyrene
	2,3-Phenylenepyrene
	IP
	Indenopyrene
	Rcra waste number U137
	o-phenylenepyrene
Inchi:	InChI=1S/C22H12/c1-2-7-17-16(6-1)18-11-10-14-9-8-13-4-3-5-15-12-19(17)22(18)21(14)
InchiKey:	SXQBHARYMNFBPS-UHFFFAOYSA-N
Formula:	C22H12
SMILES:	c1ccc2c(c1)-c1ccc3ccc4cccc5cc-2c1c3c45
Mol. weight [g/mol]:	276.33
CAS:	193-39-5

Physical Properties

Property code	Value	Unit	Source
gf	729.98	kJ/mol	Joback Method
hf	557.67	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Solid vapor pressure for five heavy PAHs via the Knudsen effusion method
hvap	76.42	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	6.231		Crippen Method
mcvol	208.380	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	3096.00		NIST Webbook
rinpol	3063.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3086.00		NIST Webbook
rinpol	3086.00		NIST Webbook
rinpol	3131.00		NIST Webbook
rinpol	495.90		NIST Webbook
rinpol	495.30		NIST Webbook

rinpol	493.65		NIST Webbook
rinpol	493.82		NIST Webbook
rinpol	492.36		NIST Webbook
rinpol	491.41		NIST Webbook
rinpol	491.35		NIST Webbook
rinpol	488.90		NIST Webbook
rinpol	493.88		NIST Webbook
rinpol	489.49		NIST Webbook
rinpol	493.24		NIST Webbook
rinpol	481.87		NIST Webbook
rinpol	3081.00		NIST Webbook
rinpol	494.91		NIST Webbook
rinpol	493.24		NIST Webbook
rinpol	493.88		NIST Webbook
rinpol	494.91		NIST Webbook
rinpol	488.60		NIST Webbook
rinpol	490.26		NIST Webbook
rinpol	490.69		NIST Webbook
rinpol	487.14		NIST Webbook
rinpol	493.30		NIST Webbook
rinpol	490.69		NIST Webbook
rinpol	490.80		NIST Webbook
rinpol	493.59		NIST Webbook
rinpol	495.80		NIST Webbook
rinpol	3082.00		NIST Webbook
rinpol	491.28		NIST Webbook
rinpol	495.71		NIST Webbook
rinpol	3081.00		NIST Webbook
rinpol	3131.00		NIST Webbook
rinpol	3131.00		NIST Webbook
rinpol	486.60		NIST Webbook
rinpol	481.87		NIST Webbook
tb	828.86	K	Joback Method
tc	1092.51	K	Joback Method
tf	437.70 ± 0.60	K	NIST Webbook
tf	435.00 ± 1.00	K	NIST Webbook
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	573.06	J/mol×K	828.86	Joback Method
cpg	586.21	J/mol×K	872.80	Joback Method
cpg	599.31	J/mol×K	916.74	Joback Method
cpg	612.69	J/mol×K	960.68	Joback Method
cpg	626.73	J/mol×K	1004.62	Joback Method
cpg	641.76	J/mol×K	1048.57	Joback Method
cpg	658.14	J/mol×K	1092.51	Joback Method
dvisc	0.0083273	Pa×s	630.03	Joback Method
dvisc	0.0083814	Pa×s	590.26	Joback Method
dvisc	0.0082799	Pa×s	669.79	Joback Method
dvisc	0.0082380	Pa×s	709.56	Joback Method
dvisc	0.0082008	Pa×s	749.33	Joback Method
dvisc	0.0081674	Pa×s	789.09	Joback Method
dvisc	0.0081374	Pa×s	828.86	Joback Method
hfust	18.60	kJ/mol	437.00	NIST Webbook
hfust	21.51	kJ/mol	435.20	NIST Webbook
hfust	21.51	kJ/mol	435.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C193395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid vapor pressure for five heavy PAHs via the Knudsen effusion method:	https://www.doi.org/10.1016/j.jct.2011.05.030
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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