Benzo[b]chrysene

Other names:	Benzo[c]tetraphene
	Dibenzo-2,3,7,8-phenanthrene
	2,3-Benzochrysene
	2,3:7,8-Dibenzophenanthrene
	3,4-Benzotetraphene
	1,2:6,7-Dibenzophenanthrene
	3,4-Benztetraphene
	Naphth(2,1-a)anthracene
	2,3-Benzchrysene
	3,4-Benzotetracene
	NSC 89274
Inchi:	InChI=1S/C22H14/c1-2-7-17-14-22-18(13-16(17)6-1)10-12-20-19-8-4-3-5-15(19)9-11-21(
InchiKey:	YYGRIGYJXSQDQB-UHFFFAOYSA-N
Formula:	C22H14
SMILES:	c1ccc2cc3c(ccc4c5ccccc5ccc34)cc2c1
Mol. weight [g/mol]:	278.35
CAS:	214-17-5

Physical Properties

Property code	Value	Unit	Source
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	7.29	eV	NIST Webbook
ie	7.14 ± 0.04	eV	NIST Webbook
ie	7.20 ± 0.02	eV	NIST Webbook
log10ws	-8.69		Crippen Method
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	498.84		NIST Webbook
rinpol	498.84		NIST Webbook
rinpol	498.86		NIST Webbook
rinpol	493.50		NIST Webbook
rinpol	496.07		NIST Webbook
rinpol	497.70		NIST Webbook

rinpol	498.50		NIST Webbook
rinpol	496.78		NIST Webbook
rinpol	496.94		NIST Webbook
rinpol	496.65		NIST Webbook
rinpol	497.66		NIST Webbook
rinpol	497.66		NIST Webbook
rinpol	3159.00		NIST Webbook
rinpol	498.86		NIST Webbook
rinpol	496.07		NIST Webbook
rinpol	496.65		NIST Webbook
rinpol	498.84		NIST Webbook
rinpol	498.50		NIST Webbook
rinpol	498.86		NIST Webbook
rinpol	497.66		NIST Webbook
rinpol	498.90		NIST Webbook
rinpol	497.66		NIST Webbook
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
rinpol	498.50		NIST Webbook
rinpol	496.50		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	567.00 ± 5.00	K	NIST Webbook
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method
hfust	25.30	kJ/mol	574.20	NIST Webbook
hsubt	136.90	kJ/mol	455.50	NIST Webbook
hsubt	136.40	kJ/mol	417.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C214175&Units=SI
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

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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