Benzo[c]phenanthrene

Other names:	3,4-Benzophenanthrene
	Benzo-3,4-phenanthrene
	Tetrahelicene
	3,4-Benzphenanthrene
Inchi:	InChI=1S/C18H12/c1-3-7-16-13(5-1)9-11-15-12-10-14-6-2-4-8-17(14)18(15)16/h1-12H
InchiKey:	TUAHORSUHVUKBD-UHFFFAOYSA-N
Formula:	C18H12
SMILES:	c1ccc2c(c1)ccc1ccc3ccccc3c12
Mol. weight [g/mol]:	228.29
CAS:	195-19-7

Physical Properties

Property code	Value	Unit	Source
chs	-8983.00 ± 1.90	kJ/mol	NIST Webbook
ea	0.55 ± 0.01	eV	NIST Webbook
ea	0.33	eV	NIST Webbook
gf	513.78	kJ/mol	Joback Method
hf	291.20	kJ/mol	NIST Webbook
hfs	184.90 ± 3.00	kJ/mol	NIST Webbook
hfus	26.70	kJ/mol	Joback Method
hsub	106.00	kJ/mol	NIST Webbook
hsub	106.30	kJ/mol	NIST Webbook
hvap	64.18	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.62	eV	NIST Webbook
ie	7.86	eV	NIST Webbook
ie	7.76	eV	NIST Webbook
ie	7.60 ± 0.02	eV	NIST Webbook
log10ws	-6.88		Crippen Method
logp	5.146		Crippen Method
mcvol	182.340	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	390.27		NIST Webbook
rinpol	391.39		NIST Webbook
rinpol	2400.20		NIST Webbook
rinpol	2427.00		NIST Webbook

rinpol	2427.00		NIST Webbook
rinpol	2400.20		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	391.30		NIST Webbook
rinpol	391.11		NIST Webbook
rinpol	391.07		NIST Webbook
rinpol	390.89		NIST Webbook
rinpol	391.12		NIST Webbook
rinpol	394.30		NIST Webbook
rinpol	391.07		NIST Webbook
rinpol	391.24		NIST Webbook
rinpol	391.39		NIST Webbook
rinpol	390.90		NIST Webbook
rinpol	390.57		NIST Webbook
rinpol	390.57		NIST Webbook
rinpol	391.07		NIST Webbook
rinpol	391.24		NIST Webbook
rinpol	389.36		NIST Webbook
rinpol	391.10		NIST Webbook
rinpol	389.52		NIST Webbook
rinpol	388.58		NIST Webbook
rinpol	389.97		NIST Webbook
tb	704.82	K	Joback Method
tc	968.39	K	Joback Method
tf	341.00 ± 1.00	K	NIST Webbook
tf	342.00 ± 1.00	K	NIST Webbook
tf	334.80 ± 0.80	K	NIST Webbook
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.24	J/mol×K	968.39	Joback Method
cpg	468.00	J/mol×K	704.82	Joback Method
cpg	482.86	J/mol×K	748.75	Joback Method
cpg	496.51	J/mol×K	792.68	Joback Method
cpg	509.15	J/mol×K	836.61	Joback Method
cpg	521.02	J/mol×K	880.54	Joback Method

cpg	532.31	J/mol×K	924.47	Joback Method
dvisc	0.0007153	Pa×s	704.82	Joback Method
dvisc	0.0017235	Pa×s	442.18	Joback Method
dvisc	0.0013935	Pa×s	485.95	Joback Method
dvisc	0.0011669	Pa×s	529.73	Joback Method
dvisc	0.0010040	Pa×s	573.50	Joback Method
dvisc	0.0008825	Pa×s	617.27	Joback Method
dvisc	0.0007890	Pa×s	661.05	Joback Method
hfust	16.32	kJ/mol	334.70	NIST Webbook
hfust	15.50	kJ/mol	339.20	NIST Webbook
hfust	16.32	kJ/mol	334.70	NIST Webbook
hsubt	106.00	kJ/mol	293.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C195197&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

chs: Standard solid enthalpy of combustion
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
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
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