Benzo[j]fluoranthene

Other names:	205-82-3
	7,8-Benzofluoranthene
	B(j)F
	Benz(j)fluoranthene
	Benzo(j)fluoranthene
	Benzo[l]fluoranthene
	Dibenzo[a,jk]fluorene
Inchi:	InChI=1S/C20H12/c1-2-8-15-13(5-1)11-12-17-16-9-3-6-14-7-4-10-18(19(14)16)20(15)17/
InchiKey:	KHNYNFUTFKJLDD-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1ccc2c3c(ccc2c1)-c1cccc2cccc-3c12
Mol. weight [g/mol]:	252.31
CAS:	205-82-3

Physical Properties

Property code	Value	Unit	Source
gf	621.88	kJ/mol	Joback Method
hf	464.81	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Joback Method
log10ws	-8.00		Aqueous Solubility Prediction Method
log10ws	-8.00		Estimated Solubility Method
logp	5.640		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	443.64		NIST Webbook
rinpol	2725.00		NIST Webbook
rinpol	2704.00		NIST Webbook
rinpol	440.92		NIST Webbook
rinpol	443.19		NIST Webbook
rinpol	444.06		NIST Webbook
rinpol	442.45		NIST Webbook
rinpol	432.90		NIST Webbook
rinpol	432.90		NIST Webbook
rinpol	2711.00		NIST Webbook

rinpol	2756.00		NIST Webbook
rinpol	443.13		NIST Webbook
rinpol	440.92		NIST Webbook
rinpol	430.60		NIST Webbook
rinpol	440.90		NIST Webbook
rinpol	442.35		NIST Webbook
rinpol	440.92		NIST Webbook
rinpol	440.92		NIST Webbook
rinpol	440.92		NIST Webbook
rinpol	430.60		NIST Webbook
rinpol	440.92		NIST Webbook
rinpol	2756.00		NIST Webbook
rinpol	2704.00		NIST Webbook
rinpol	441.95		NIST Webbook
tb	766.84	K	Joback Method
tc	1030.60	K	Joback Method
tf	516.22	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.16	J/mol×K	766.84	Joback Method
cpg	534.69	J/mol×K	810.80	Joback Method
cpg	547.49	J/mol×K	854.76	Joback Method
cpg	559.83	J/mol×K	898.72	Joback Method
cpg	572.01	J/mol×K	942.68	Joback Method
cpg	584.31	J/mol×K	986.64	Joback Method
cpg	597.00	J/mol×K	1030.60	Joback Method
dvisc	0.0032474	Pa×s	516.22	Joback Method
dvisc	0.0029976	Pa×s	557.99	Joback Method
dvisc	0.0027980	Pa×s	599.76	Joback Method
dvisc	0.0026352	Pa×s	641.53	Joback Method
dvisc	0.0025002	Pa×s	683.30	Joback Method
dvisc	0.0023865	Pa×s	725.07	Joback Method
dvisc	0.0022895	Pa×s	766.84	Joback Method
hfust	17.90	kJ/mol	438.30	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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=C205823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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