Benzo(a)fluoranthene

Other names:	1,2-benzfluoranthene
	1,2-Benzofluoranthene
	Benz[a]aceanthrylene
Inchi:	InChI=1S/C20H12/c1-2-8-15-13(6-1)12-14-7-5-11-17-16-9-3-4-10-18(16)20(15)19(14)17/
InchiKey:	OQDXASJSCOTNQS-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	c1ccc2c(c1)-c1cccc3cc4ccccc4c-2c13
Mol. weight [g/mol]:	252.31
CAS:	203-33-8

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	-8.53		Crippen Method
logp	5.640		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
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

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C203338&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume