Benz[l]aceanthrylene

Inchi: InChI=1S/C20H12/c1-2-7-17-13(4-1)8-9-16-12-15-6-3-5-14-10-11-18(19(14)15)20(16)17/
InchiKey: ICRHCNSZHYPRNZ-UHFFFAOYSA-N
Formula: C20H12
SMILES: C1=Cc2c3c1cccc3cc1ccc3ccccc3c21
Mol. weight [g/mol]: 252.31
CAS: 211-91-6

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	-7.74		Crippen Method
logp	5.630		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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C211916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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