Benzo[a]pyrene, 4,5-dihydro-

Other names: 4,5-Dihydrobenzo(a)pyrene
Inchi: InChI=1S/C20H14/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14/
InchiKey: WMXZGBBYGZWMCZ-UHFFFAOYSA-N
Formula: C20H14
SMILES: c1ccc2c(c1)cc1c3c2ccc2cccc(c23)CC1
Mol. weight [g/mol]: 254.33
CAS: 57652-66-1

Physical Properties

Property code	Value	Unit	Source
gf	591.92	kJ/mol	Joback Method
hf	407.03	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	5.245		Crippen Method
mcvol	199.660	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
tb	767.68	K	Joback Method
tc	1029.07	K	Joback Method
tf	515.46	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.24	J/mol×K	767.68	Joback Method
cpg	561.86	J/mol×K	811.24	Joback Method
cpg	575.67	J/mol×K	854.81	Joback Method
cpg	588.96	J/mol×K	898.37	Joback Method
cpg	601.98	J/mol×K	941.94	Joback Method
cpg	615.02	J/mol×K	985.50	Joback Method
cpg	628.35	J/mol×K	1029.07	Joback Method
dvisc	0.0032582	Pa×s	515.46	Joback Method

dvisc	0.0029636	Pa×s	557.50	Joback Method
dvisc	0.0027317	Pa×s	599.53	Joback Method
dvisc	0.0025450	Pa×s	641.57	Joback Method
dvisc	0.0023918	Pa×s	683.61	Joback Method
dvisc	0.0022640	Pa×s	725.64	Joback Method
dvisc	0.0021560	Pa×s	767.68	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=C57652661&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