Naphtho[1,2-a]anthracene

Other names: 2,3:5,6-Dibenzophenanthrene
Dibenzo[b,g]phenanthrene
Inchi: InChI=1S/C22H14/c1-2-7-18-14-21-19(13-17(18)6-1)12-11-16-10-9-15-5-3-4-8-20(15)22(
InchiKey: HAJMQPPSPOBCLG-UHFFFAOYSA-N
Formula: C22H14
SMILES: c1ccc2cc3c(ccc4ccc5ccccc5c43)cc2c1
Mol. weight [g/mol]: 278.35
CAS: 195-06-2

Physical Properties

Property code	Value	Unit	Source
gf	644.48	kJ/mol	Joback Method
hf	468.99	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
ie	7.33	eV	NIST Webbook
ie	7.11	eV	NIST Webbook
log10ws	-8.69		Crippen Method
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	485.71		NIST Webbook
rinpol	485.71		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	532.48	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.64	J/mol×K	820.30	Joback Method
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method

cpg	650.13	J/mol×K	955.09	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method
dvisc	0.0022584	Pa×s	532.48	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C195062&Units=SI

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
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