6H-Benzo[cd]pyrene

Inchi: InChI=1S/C19H12/c1-3-12-7-9-14-10-8-13-4-2-6-16-11-15(5-1)17(12)19(14)18(13)16/h1-
InchiKey: CFXWAPSYPXUYCO-UHFFFAOYSA-N
Formula: C19H12
SMILES: c1cc2c3c(c1)ccc1ccc4cccc(c4c13)C2
Mol. weight [g/mol]: 240.30
CAS: 191-33-3

Physical Properties

Property code	Value	Unit	Source
gf	595.60	kJ/mol	Joback Method
hf	433.83	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	5.050		Crippen Method
mcvol	185.570	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	740.53	K	Joback Method
tc	999.94	K	Joback Method
tf	408.00 ± 4.00	K	NIST Webbook
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.08	J/mol×K	740.53	Joback Method
cpg	553.80	J/mol×K	956.70	Joback Method
cpg	541.90	J/mol×K	913.47	Joback Method
cpg	530.06	J/mol×K	870.23	Joback Method
cpg	517.99	J/mol×K	827.00	Joback Method
cpg	505.43	J/mol×K	783.76	Joback Method
cpg	566.02	J/mol×K	999.94	Joback Method
dvisc	0.0030808	Pa×s	740.53	Joback Method
dvisc	0.0031601	Pa×s	701.73	Joback Method

dvisc	0.0032511	Pa×s	662.92	Joback Method
dvisc	0.0033565	Pa×s	624.12	Joback Method
dvisc	0.0034800	Pa×s	585.32	Joback Method
dvisc	0.0036267	Pa×s	546.51	Joback Method
dvisc	0.0038035	Pa×s	507.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C191333&Units=SI

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

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