Hexahelicene

Other names: Phenanthro[3,4-c]phenanthrene
[6]Helicene
Inchi: InChI=1S/C26H16/c1-3-7-22-17(5-1)9-11-19-13-15-21-16-14-20-12-10-18-6-2-4-8-23(18)
InchiKey: UOYPNWSDSPYOSN-UHFFFAOYSA-N
Formula: C26H16
SMILES: c1ccc2c(c1)ccc1ccc3ccc4ccc5ccccc5c4c3c12
Mol. weight [g/mol]: 328.41
CAS: 187-83-7

Physical Properties

Property code	Value	Unit	Source
gf	775.18	kJ/mol	Joback Method
hf	566.03	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
ie	7.37	eV	NIST Webbook
ie	7.37	eV	NIST Webbook
log10ws	-10.49		Crippen Method
logp	7.453		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	3335.00		NIST Webbook
rinpol	509.74		NIST Webbook
rinpol	509.79		NIST Webbook
rinpol	3260.00		NIST Webbook
rinpol	3320.00		NIST Webbook
rinpol	3335.00		NIST Webbook
rinpol	3260.00		NIST Webbook
rinpol	3320.00		NIST Webbook
rinpol	3335.00		NIST Webbook
rinpol	3260.00		NIST Webbook
tb	935.78	K	Joback Method
tc	1209.93	K	Joback Method
tf	622.78	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.48	J/mol×K	935.78	Joback Method
cpg	769.57	J/mol×K	981.47	Joback Method
cpg	785.72	J/mol×K	1027.16	Joback Method
cpg	802.30	J/mol×K	1072.85	Joback Method
cpg	819.68	J/mol×K	1118.55	Joback Method
cpg	838.20	J/mol×K	1164.24	Joback Method
cpg	858.23	J/mol×K	1209.93	Joback Method
dvisc	0.0031676	Pa×s	622.78	Joback Method
dvisc	0.0027637	Pa×s	674.95	Joback Method
dvisc	0.0024589	Pa×s	727.11	Joback Method
dvisc	0.0022223	Pa×s	779.28	Joback Method
dvisc	0.0020341	Pa×s	831.45	Joback Method
dvisc	0.0018814	Pa×s	883.61	Joback Method
dvisc	0.0017553	Pa×s	935.78	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=C187837&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
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