[14]Helicene

Other names: Diphenanthro[4,3-g:4',3'-g']naphtho[2,1-c:7,8-c']diphenanthrene
Inchi: InChI=1S/C58H32/c1-3-7-46-33(5-1)9-11-35-13-15-37-17-19-39-21-23-41-25-27-43-29-3
InchiKey: FYHJTLVERBIHKT-UHFFFAOYSA-N
Formula: C58H32
SMILES: c1ccc2c(c1)ccc1ccc3ccc4ccc5ccc6ccc7ccc8ccc9ccc%10ccc%11ccc%12ccc%13ccccc%
Mol. weight [g/mol]: 728.87
CAS: 57483-71-3

Physical Properties

Property code	Value	Unit	Source
gf	1820.78	kJ/mol	Joback Method
hf	1342.35	kJ/mol	Joback Method
hfus	96.60	kJ/mol	Joback Method
hvap	176.24	kJ/mol	Joback Method
ie	6.88	eV	NIST Webbook
log10ws	-24.93		Crippen Method
logp	16.678		Crippen Method
mcvol	551.340	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
tb	1859.62	K	Joback Method
tc	2342.70	K	Joback Method
tf	1345.18	K	Joback Method
vc	2.162	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3456.59	J/mol×K	1859.62	Joback Method
cpg	3840.73	J/mol×K	1940.13	Joback Method
cpg	4281.43	J/mol×K	2020.65	Joback Method
cpg	4783.25	J/mol×K	2101.16	Joback Method
cpg	5350.77	J/mol×K	2181.67	Joback Method
cpg	5988.57	J/mol×K	2262.19	Joback Method
cpg	6701.21	J/mol×K	2342.70	Joback Method

dvisc	0.0925601	Pa×s	1345.18	Joback Method
dvisc	0.0872679	Pa×s	1430.92	Joback Method
dvisc	0.0828278	Pa×s	1516.66	Joback Method
dvisc	0.0790542	Pa×s	1602.40	Joback Method
dvisc	0.0758107	Pa×s	1688.14	Joback Method
dvisc	0.0729954	Pa×s	1773.88	Joback Method
dvisc	0.0705303	Pa×s	1859.62	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=C57483713&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume