Phenanthro[3,4-c]phenanthrene

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

Physical Properties

Property code	Value	Unit	Source
af	0.6664		Cheméo Relay (1.0)
gf	775.18	kJ/mol	Joback Method
hf	454.72	kJ/mol	Cheméo Relay (1.0)
hfus	40.68	kJ/mol	Joback Method
hvap	147.54	kJ/mol	Cheméo Relay (1.0)
ie	7.37	eV	NIST Webbook
ie	7.37	eV	NIST Webbook
log10ws	-9.23		Cheméo Relay (1.0)
logp	7.453		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	3320.00		NIST Webbook
rinpol	509.74		NIST Webbook
rinpol	3335.00		NIST Webbook
rinpol	3260.00		NIST Webbook
rinpol	3320.00		NIST Webbook
rinpol	3335.00		NIST Webbook
rinpol	509.79		NIST Webbook
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook
rinpol	3335.00		NIST Webbook
tb	844.07	K	Cheméo Relay (1.0)
tc	1197.06	K	Cheméo Relay (1.0)
tf	514.50	K	Cheméo Relay (1.0)
vc	0.973	m3/kmol	Cheméo Relay (1.0)

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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C187837&Units=SI

Legend

af: Acentric Factor
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