

Hexaphene

Inchi:	InChI=1S/C26H16/c1-2-7-19-13-24-16-26-22(14-23(24)12-18(19)6-1)10-9-21-11-17-5-3-
InchiKey:	PKIFBGYEEVFWTJ-UHFFFAOYSA-N
Formula:	C26H16
SMILES:	<chem>c1ccc2cc3cc4c(ccc5cc6ccccc6cc54)cc3cc2c1</chem>
Mol. weight [g/mol]:	328.41
CAS:	222-78-6

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	7.09	eV	NIST Webbook
ie	7.02 ± 0.04	eV	NIST Webbook
ie	6.92 ± 0.02	eV	NIST Webbook
ie	6.81	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	618.78		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	620.00		NIST Webbook
tb	935.78	K	Joback Method
tc	1209.93	K	Joback Method
tf	622.78	K	Joback Method
vc	0.994	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.48	J/mol×K	935.78	Joback Method
cpg	838.20	J/mol×K	1164.24	Joback Method

cpg	819.68	J/molxK	1118.55	Joback Method
cpg	802.30	J/molxK	1072.85	Joback Method
cpg	785.72	J/molxK	1027.16	Joback Method
cpg	769.57	J/molxK	981.47	Joback Method
cpg	858.23	J/molxK	1209.93	Joback Method
dvisc	0.0017553	Paxs	935.78	Joback Method
dvisc	0.0018814	Paxs	883.61	Joback Method
dvisc	0.0020341	Paxs	831.45	Joback Method
dvisc	0.0022223	Paxs	779.28	Joback Method
dvisc	0.0024589	Paxs	727.11	Joback Method
dvisc	0.0027637	Paxs	674.95	Joback Method
dvisc	0.0031676	Paxs	622.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C222786&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
hvac:	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

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