[9]Helicene

Other names: Diphenanthro[3,4-c:4'3'-g]phenanthrene
Inchi: InChI=1S/C38H22/c1-3-7-31-23(5-1)9-11-25-13-15-27-17-19-29-21-22-30-20-18-28-16-1
InchiKey: LKCSSGNXXHZCJW-UHFFFAOYSA-N
Formula: C38H22
SMILES: c1ccc2c(c1)ccc1ccc3ccc4ccc5ccc6ccc7ccc8ccccc8c7c6c5c4c3c12
Mol. weight [g/mol]: 478.58
CAS: 20495-14-1

Physical Properties

Property code	Value	Unit	Source
gf	1167.28	kJ/mol	Joback Method
hf	857.15	kJ/mol	Joback Method
hfus	61.65	kJ/mol	Joback Method
hvap	120.21	kJ/mol	Joback Method
ie	7.07	eV	NIST Webbook
ie	7.07	eV	NIST Webbook
log10ws	-15.91		Crippen Method
logp	10.912		Crippen Method
mcvol	366.840	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
tb	1282.22	K	Joback Method
tc	1580.19	K	Joback Method
tf	893.68	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.69	J/mol×K	1282.22	Joback Method
cpg	1332.23	J/mol×K	1331.88	Joback Method
cpg	1379.99	J/mol×K	1381.54	Joback Method
cpg	1433.68	J/mol×K	1431.21	Joback Method
cpg	1493.99	J/mol×K	1480.87	Joback Method
cpg	1561.60	J/mol×K	1530.53	Joback Method

cpg	1637.22	J/mol×K	1580.19	Joback Method
dvisc	0.0104640	Pa×s	893.68	Joback Method
dvisc	0.0095691	Pa×s	958.44	Joback Method
dvisc	0.0088502	Pa×s	1023.19	Joback Method
dvisc	0.0082618	Pa×s	1087.95	Joback Method
dvisc	0.0077724	Pa×s	1152.71	Joback Method
dvisc	0.0073596	Pa×s	1217.46	Joback Method
dvisc	0.0070073	Pa×s	1282.22	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20495141&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
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

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