

Dibenzo[q,vwx]hexaphene

Inchi:	InChI=1S/C32H18/c1-3-7-25-19(5-1)9-10-21-16-24-17-23-12-11-22-15-20-6-2-4-8-26(20)
InchiKey:	MANCMEZMBIROHA-UHFFFAOYSA-N
Formula:	C32H18
SMILES:	<chem>c1ccc2c(c1)ccc1cc3cc4ccc5cc6ccccc6c6ccc(c3cc12)c4c56</chem>
Mol. weight [g/mol]:	402.49
CAS:	119000-39-4

Physical Properties

Property code	Value	Unit	Source
gf	1013.98	kJ/mol	Joback Method
hf	755.93	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	103.92	kJ/mol	Joback Method
log10ws	-13.52		Crippen Method
logp	9.197		Crippen Method
mcvol	306.060	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	1113.28	K	Joback Method
tc	1393.93	K	Joback Method
tf	787.12	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.19	J/molxK	1113.28	Joback Method
cpg	1141.24	J/molxK	1347.16	Joback Method
cpg	1101.51	J/molxK	1300.38	Joback Method
cpg	1066.07	J/molxK	1253.61	Joback Method
cpg	1034.40	J/molxK	1206.83	Joback Method
cpg	1005.95	J/molxK	1160.06	Joback Method
cpg	1185.80	J/molxK	1393.93	Joback Method
dvisc	0.0110928	Paxs	1113.28	Joback Method
dvisc	0.0114227	Paxs	1058.92	Joback Method

dvisc	0.0117997	Paxs	1004.56	Joback Method
dvisc	0.0122346	Paxs	950.20	Joback Method
dvisc	0.0127414	Paxs	895.84	Joback Method
dvisc	0.0133389	Paxs	841.48	Joback Method
dvisc	0.0140531	Paxs	787.12	Joback Method

Sources

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=C119000394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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