DIBENZO[J,XYZ]HEPTAPHENE

Inchi: InChI=1S/C36H20/c1-3-9-23-17-31-25(15-21(23)7-1)19-33-27-11-5-6-12-28(27)34-20-26
InchiKey: KADSIADUIOVQLQ-UHFFFAOYSA-N
Formula: C36H20
SMILES: c1ccc2cc3c(cc2c1)cc1c2ccccc2c2cc4cc5ccccc5cc4c4ccc3c1c42
Mol. weight [g/mol]: 452.56

Physical Properties

Property code	Value	Unit	Source
hf	596.09	kJ/mol	Cheméo Relay (1.0)
hfus	59.44	kJ/mol	Joback Method
hvap	216.47	kJ/mol	Cheméo Relay (1.0)
ie	6.74	eV	NIST Webbook
log10ws	-14.18		Cheméo Relay (1.0)
logp	10.350		Crippen Method
mcvol	342.960	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
tb	1048.93	K	Cheméo Relay (1.0)
tc	1462.96	K	Cheméo Relay (1.0)
tf	695.03	K	Cheméo Relay (1.0)
vc	1.327	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.13	J/mol×K	1228.76	Joback Method
cpg	1214.90	J/mol×K	1277.19	Joback Method
cpg	1258.52	J/mol×K	1325.61	Joback Method
cpg	1307.64	J/mol×K	1374.04	Joback Method
cpg	1362.92	J/mol×K	1422.46	Joback Method
cpg	1425.02	J/mol×K	1470.89	Joback Method
cpg	1494.62	J/mol×K	1519.31	Joback Method
dvisc	0.0228438	Pa×s	877.42	Joback Method
dvisc	0.0217885	Pa×s	935.98	Joback Method
dvisc	0.0208980	Pa×s	994.53	Joback Method

dvisc	0.0201371	Pa×s	1053.09	Joback Method
dvisc	0.0194799	Pa×s	1111.65	Joback Method
dvisc	0.0189069	Pa×s	1170.20	Joback Method
dvisc	0.0184030	Pa×s	1228.76	Joback Method

Sources

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=C192461&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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