DIBENZO[A,J]CORONENE

Inchi: InChI=1S/C32H16/c1-2-6-20-19(5-1)23-13-9-17-11-15-25-21-7-3-4-8-22(21)26-16-12-18-
InchiKey: HHCCABYUXOGSCO-UHFFFAOYSA-N
Formula: C32H16
SMILES: c1ccc2c(c1)c1ccc3ccc4c5ccccc5c5ccc6ccc2c2c6c5c4c3c12
Mol. weight [g/mol]: 400.48

Physical Properties

Property code	Value	Unit	Source
hf	574.85	kJ/mol	Cheméo Relay (1.0)
hfus	55.04	kJ/mol	Joback Method
hvap	196.15	kJ/mol	Cheméo Relay (1.0)
ie	6.92	eV	NIST Webbook
ie	6.92	eV	NIST Webbook
ie	6.92	eV	NIST Webbook
log10ws	-12.19		Cheméo Relay (1.0)
logp	9.226		Crippen Method
mcvol	295.200	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
tb	976.47	K	Cheméo Relay (1.0)
tc	1395.73	K	Cheméo Relay (1.0)
tf	647.31	K	Cheméo Relay (1.0)
vc	1.210	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.39	J/mol×K	1121.84	Joback Method
cpg	1209.85	J/mol×K	1399.15	Joback Method
cpg	1152.95	J/mol×K	1352.93	Joback Method
cpg	1102.53	J/mol×K	1306.71	Joback Method
cpg	1057.97	J/mol×K	1260.50	Joback Method
cpg	1018.68	J/mol×K	1214.28	Joback Method
cpg	984.02	J/mol×K	1168.06	Joback Method
dvisc	0.1074272	Pa×s	983.37	Joback Method

dvisc	0.1126083	Pa×s	1121.84	Joback Method
dvisc	0.1110035	Pa×s	1075.68	Joback Method
dvisc	0.1092809	Pa×s	1029.53	Joback Method
dvisc	0.1009143	Pa×s	844.90	Joback Method
dvisc	0.1054271	Pa×s	937.21	Joback Method
dvisc	0.1032630	Pa×s	891.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C190727&Units=SI
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):	

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