

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]:	400.47
CAS:	190-72-7

Physical Properties

Property code	Value	Unit	Source
gf	1099.48	kJ/mol	Joback Method
hf	844.61	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	104.95	kJ/mol	Joback Method
ie	6.92	eV	NIST Webbook
ie	6.92	eV	NIST Webbook
ie	6.92	eV	NIST Webbook
log10ws	-14.15		Crippen Method
logp	9.226		Crippen Method
mcvol	295.200	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
tb	1121.84	K	Joback Method
tc	1399.15	K	Joback Method
tf	844.90	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.39	J/molxK	1121.84	Joback Method
cpg	984.02	J/molxK	1168.06	Joback Method
cpg	1018.68	J/molxK	1214.28	Joback Method
cpg	1057.97	J/molxK	1260.50	Joback Method
cpg	1102.53	J/molxK	1306.71	Joback Method
cpg	1152.95	J/molxK	1352.93	Joback Method

cpg	1209.85	J/mol×K	1399.15	Joback Method
dvisc	0.1009143	Paxs	844.90	Joback Method
dvisc	0.1032630	Paxs	891.06	Joback Method
dvisc	0.1054271	Paxs	937.21	Joback Method
dvisc	0.1074272	Paxs	983.37	Joback Method
dvisc	0.1092809	Paxs	1029.53	Joback Method
dvisc	0.1110035	Paxs	1075.68	Joback Method
dvisc	0.1126083	Paxs	1121.84	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=C190727&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
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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