

1,2-Dihydrobenz[j]aceanthrylene

Other names:	1,2-Dihydrobenz[j]aceanthrylene 479-23-2 cholanthrene
Inchi:	InChI=1S/C20H14/c1-2-7-16-13(4-1)8-10-17-18-11-9-14-5-3-6-15(20(14)18)12-19(16)17
InchiKey:	KVFJBIQWENJTDM-UHFFFAOYSA-N
Formula:	C20H14
SMILES:	<chem>c1cc2c3c(c4ccc5ccccc5c4cc3c1)CC2</chem>
Mol. weight [g/mol]:	254.33
CAS:	479-23-2

Physical Properties

Property code	Value	Unit	Source
gf	591.92	kJ/mol	Joback Method
hf	407.03	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-7.85		Aqueous Solubility Prediction Method
log10ws	-7.85		Estimated Solubility Method
logp	5.245		Crippen Method
mcvol	199.660	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
tb	767.68	K	Joback Method
tc	1029.07	K	Joback Method
tf	515.46	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.24	J/mol×K	767.68	Joback Method
cpg	561.86	J/mol×K	811.24	Joback Method
cpg	575.67	J/mol×K	854.81	Joback Method

cpg	588.96	J/mol×K	898.37	Joback Method
cpg	601.98	J/mol×K	941.94	Joback Method
cpg	615.02	J/mol×K	985.50	Joback Method
cpg	628.35	J/mol×K	1029.07	Joback Method
dvisc	0.0032582	Paxs	515.46	Joback Method
dvisc	0.0029636	Paxs	557.50	Joback Method
dvisc	0.0027317	Paxs	599.53	Joback Method
dvisc	0.0025450	Paxs	641.57	Joback Method
dvisc	0.0023918	Paxs	683.61	Joback Method
dvisc	0.0022640	Paxs	725.64	Joback Method
dvisc	0.0021560	Paxs	767.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C479232&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
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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