

15H-Cyclopenta[a]phenanthrene

Inchi:	InChI=1S/C17H12/c1-2-6-14-12(4-1)8-10-17-15-7-3-5-13(15)9-11-16(14)17/h1-6,8-11H,7
InchiKey:	LFVNLPNQKQNMJU-UHFFFAOYSA-N
Formula:	C17H12
SMILES:	<chem>C1=Cc2ccc3c(ccc4ccccc43)c2C1</chem>
Mol. weight [g/mol]:	216.28
CAS:	219-07-8

Physical Properties

Property code	Value	Unit	Source
gf	487.50	kJ/mol	Joback Method
hf	340.97	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.562		Crippen Method
mcvol	172.550	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	678.51	K	Joback Method
tc	937.21	K	Joback Method
tf	433.67	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.86	J/mol×K	678.51	Joback Method
cpg	502.61	J/mol×K	894.10	Joback Method
cpg	491.43	J/mol×K	850.98	Joback Method
cpg	479.68	J/mol×K	807.86	Joback Method
cpg	467.14	J/mol×K	764.74	Joback Method
cpg	453.60	J/mol×K	721.63	Joback Method
cpg	513.42	J/mol×K	937.21	Joback Method
dvisc	0.0009629	Paxs	678.51	Joback Method
dvisc	0.0010415	Paxs	637.70	Joback Method

dvisc	0.0011386	Paxs	596.90	Joback Method
dvisc	0.0012612	Paxs	556.09	Joback Method
dvisc	0.0014198	Paxs	515.28	Joback Method
dvisc	0.0016313	Paxs	474.48	Joback Method
dvisc	0.0019238	Paxs	433.67	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=C219078&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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