cis-Phenanthrene, 9,10-dihydro-9,10-diol, diacetate

Inchi: InChI=1S/C18H16O4/c1-11(19)21-17-15-9-5-3-7-13(15)14-8-4-6-10-16(14)18(17)22-12(2

InchiKey: AFGAFKSFAIFLNO-HDICACEKSA-N

Formula: C18H16O4

SMILES: CC(=O)OC1c2ccccc2-c2ccccc2C1OC(C)=O

Mol. weight [g/mol]: 296.32

Physical Properties

Property code	Value	Unit	Source
gf	-96.46	kJ/mol	Joback Method
hf	-395.71	kJ/mol	Joback Method
hfus	36.56	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.576		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	2120.00		NIST Webbook
tb	824.94	K	Joback Method
tc	1060.61	K	Joback Method
tf	532.04	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.46	J/mol×K	824.94	Joback Method
cpg	664.49	J/mol×K	864.22	Joback Method
cpg	677.37	J/mol×K	903.50	Joback Method
cpg	689.15	J/mol×K	942.77	Joback Method
cpg	699.90	J/mol×K	982.05	Joback Method
cpg	709.69	J/mol×K	1021.33	Joback Method
cpg	718.58	J/mol×K	1060.61	Joback Method
dvisc	0.0013120	Pa×s	532.04	Joback Method
dvisc	0.0009984	Pa×s	580.86	Joback Method

dvisc	0.0007926	Pa×s	629.67	Joback Method
dvisc	0.0006505	Pa×s	678.49	Joback Method
dvisc	0.0005482	Pa×s	727.31	Joback Method
dvisc	0.0004720	Pa×s	776.12	Joback Method
dvisc	0.0004137	Pa×s	824.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume