

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.46	J/molxK	824.94	Joback Method
cpg	709.69	J/molxK	1021.33	Joback Method
cpg	699.90	J/molxK	982.05	Joback Method
cpg	689.15	J/molxK	942.77	Joback Method
cpg	677.37	J/molxK	903.50	Joback Method
cpg	664.49	J/molxK	864.22	Joback Method
cpg	718.58	J/molxK	1060.61	Joback Method
dvisc	0.0004137	Paxs	824.94	Joback Method
dvisc	0.0004720	Paxs	776.12	Joback Method

dvisc	0.0005482	Paxs	727.31	Joback Method
dvisc	0.0006505	Paxs	678.49	Joback Method
dvisc	0.0007926	Paxs	629.67	Joback Method
dvisc	0.0009984	Paxs	580.86	Joback Method
dvisc	0.0013120	Paxs	532.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109430&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
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

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