cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3-methoxy, diacetate

Inchi: InChI=1S/C20H20O5/c1-12(21)24-19-16-10-9-14(23-4)11-17(16)15-7-5-6-8-18(15)20(19
InchiKey: VDRBUVUVJAQGAK-UXHICEINSA-N
Formula: C20H20O5
SMILES: COc1ccc2c(c1)-c1ccccc1C(C)(OC(C)=O)C2OC(C)=O
Mol. weight [g/mol]: 340.37

Physical Properties

Property code	Value	Unit	Source
gf	-199.74	kJ/mol	Joback Method
hf	-565.44	kJ/mol	Joback Method
hfus	36.24	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	3.758		Crippen Method
mcvol	255.030	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	898.34	K	Joback Method
tc	1132.88	K	Joback Method
tf	613.23	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.03	J/mol×K	898.34	Joback Method
cpg	804.61	J/mol×K	937.43	Joback Method
cpg	820.83	J/mol×K	976.52	Joback Method
cpg	836.84	J/mol×K	1015.61	Joback Method
cpg	852.78	J/mol×K	1054.70	Joback Method
cpg	868.81	J/mol×K	1093.79	Joback Method
cpg	885.09	J/mol×K	1132.88	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=R109549&Units=SI

Legend

cpg:	Ideal gas heat capacity
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