4,5-dihydroxy-3-methoxy-9,10-dihydrophenanthre acetylated

Inchi: InChI=1S/C19H18O5/c1-11(20)23-15-6-4-5-13-7-8-14-9-10-16(22-3)19(24-12(2)21)18(14
InchiKey: FCNFMJSSXLYNNN-UHFFFAOYSA-N
Formula: C19H18O5
SMILES: COc1ccc2c(c1OC(C)=O)-c1c(cccc1OC(C)=O)CC2
Mol. weight [g/mol]: 326.34

Physical Properties

Property code	Value	Unit	Source
gf	-206.51	kJ/mol	Joback Method
hf	-542.30	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.311		Crippen Method
mcvol	240.940	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	894.52	K	Joback Method
tc	1127.33	K	Joback Method
tf	611.58	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.09	J/mol×K	894.52	Joback Method
cpg	732.81	J/mol×K	933.32	Joback Method
cpg	744.44	J/mol×K	972.12	Joback Method
cpg	755.01	J/mol×K	1010.92	Joback Method
cpg	764.58	J/mol×K	1049.72	Joback Method
cpg	773.17	J/mol×K	1088.52	Joback Method
cpg	780.83	J/mol×K	1127.33	Joback Method
dvisc	0.0006044	Pa×s	611.58	Joback Method

dvisc	0.0004624	Pa×s	658.74	Joback Method
dvisc	0.0003667	Pa×s	705.89	Joback Method
dvisc	0.0002994	Pa×s	753.05	Joback Method
dvisc	0.0002503	Pa×s	800.21	Joback Method
dvisc	0.0002135	Pa×s	847.36	Joback Method
dvisc	0.0001852	Pa×s	894.52	Joback Method

Sources

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=R273893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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