2-hydroxy-3,5-dimethoxy-9,10-dihydrophenanthre acetylated

Inchi: InChI=1S/C18H18O4/c1-11(19)22-17-9-13-8-7-12-5-4-6-15(20-2)18(12)14(13)10-16(17)2
InchiKey: MPPPUKPVQACBDB-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: COc1cc2c(cc1OC(C)=O)CCc1cccc(OC)c1-2
Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-86.01	kJ/mol	Joback Method
hf	-409.08	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	77.55	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.395		Crippen Method
mcvol	225.280	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	817.77	K	Joback Method
tc	1047.83	K	Joback Method
tf	550.38	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.62	J/mol×K	817.77	Joback Method
cpg	666.95	J/mol×K	856.11	Joback Method
cpg	680.21	J/mol×K	894.46	Joback Method
cpg	692.44	J/mol×K	932.80	Joback Method
cpg	703.69	J/mol×K	971.14	Joback Method
cpg	713.99	J/mol×K	1009.49	Joback Method
cpg	723.39	J/mol×K	1047.83	Joback Method
dvisc	0.0006403	Pa×s	550.38	Joback Method

dvisc	0.0004913	Pa×s	594.95	Joback Method
dvisc	0.0003911	Pa×s	639.51	Joback Method
dvisc	0.0003207	Pa×s	684.08	Joback Method
dvisc	0.0002695	Pa×s	728.64	Joback Method
dvisc	0.0002310	Pa×s	773.21	Joback Method
dvisc	0.0002014	Pa×s	817.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273873&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