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

Inchi: InChI=1S/C16H16O3/c1-18-14-5-3-4-10-6-7-11-8-13(17)15(19-2)9-12(11)16(10)14/h3-5,
InchiKey: FAJHDSYEKPXYHY-UHFFFAOYSA-N
Formula: C16H16O3
SMILES: COc1cc2c(cc1O)CCc1cccc(OC)c1-2
Mol. weight [g/mol]: 256.30

Physical Properties

Property code	Value	Unit	Source
gf	-13.92	kJ/mol	Joback Method
hf	-288.84	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	76.29	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.175		Crippen Method
mcvol	195.530	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	2216.00		NIST Webbook
tb	771.36	K	Joback Method
tc	1013.22	K	Joback Method
tf	554.88	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.51	J/mol×K	771.36	Joback Method
cpg	568.62	J/mol×K	811.67	Joback Method
cpg	581.97	J/mol×K	851.98	Joback Method
cpg	594.65	J/mol×K	892.29	Joback Method
cpg	606.81	J/mol×K	932.60	Joback Method
cpg	618.56	J/mol×K	972.91	Joback Method
cpg	630.02	J/mol×K	1013.22	Joback Method
dvisc	0.0001545	Pa×s	554.88	Joback Method
dvisc	0.0001000	Pa×s	590.96	Joback Method

dvisc	0.0000680	Pa×s	627.04	Joback Method
dvisc	0.0000483	Pa×s	663.12	Joback Method
dvisc	0.0000355	Pa×s	699.20	Joback Method
dvisc	0.0000269	Pa×s	735.28	Joback Method
dvisc	0.0000209	Pa×s	771.36	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=R273868&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