4,6-Diacetoxy-3-methoxyphenanthrene

Inchi: InChI=1S/C19H16O5/c1-11(20)23-15-8-6-13-4-5-14-7-9-17(22-3)19(24-12(2)21)18(14)16
InchiKey: MYOPYNHXINLPTK-UHFFFAOYSA-N
Formula: C19H16O5
SMILES: COc1ccc2ccc3ccc(OC(C)=O)cc3c2c1OC(C)=O
Mol. weight [g/mol]: 324.33

Physical Properties

Property code	Value	Unit	Source
gf	-176.55	kJ/mol	Joback Method
hf	-484.52	kJ/mol	Joback Method
hfus	38.25	kJ/mol	Joback Method
hvap	86.81	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	3.852		Crippen Method
mcvol	236.640	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
tb	893.68	K	Joback Method
tc	1127.85	K	Joback Method
tf	612.34	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.69	J/mol×K	893.68	Joback Method
cpg	702.64	J/mol×K	932.71	Joback Method
cpg	713.56	J/mol×K	971.74	Joback Method
cpg	723.48	J/mol×K	1010.76	Joback Method
cpg	732.46	J/mol×K	1049.79	Joback Method
cpg	740.54	J/mol×K	1088.82	Joback Method
cpg	747.76	J/mol×K	1127.85	Joback Method
dvisc	0.0006195	Pa×s	612.34	Joback Method

dvisc	0.0004803	Pa×s	659.23	Joback Method
dvisc	0.0003852	Pa×s	706.12	Joback Method
dvisc	0.0003175	Pa×s	753.01	Joback Method
dvisc	0.0002677	Pa×s	799.90	Joback Method
dvisc	0.0002300	Pa×s	846.79	Joback Method
dvisc	0.0002008	Pa×s	893.68	Joback Method

Sources

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=R330768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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