(17-acetyl-6-chloro-10,13-dimethyl-3-oxo-9,11,12,1 acetate

Inchi: InChI=1S/C23H27ClO4/c1-13(25)23(28-14(2)26)10-7-18-16-12-20(24)19-11-15(27)5-8-2
InchiKey: CGBCCZZJVKUAMX-UHFFFAOYSA-N
Formula: C23H27ClO4
SMILES: CC(=O)OC1(C(C)=O)CCC2C3C=C(Cl)C4=CC(=O)C=CC4(C)C3CCC21C
Mol. weight [g/mol]: 402.92

Physical Properties

Property code	Value	Unit	Source
gf	-133.35	kJ/mol	Joback Method
hf	-613.03	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	89.97	kJ/mol	Joback Method
log10ws	-4.95		Aqueous Solubility Prediction Method
logp	4.528		Crippen Method
mcvol	301.410	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
tb	1008.18	K	Joback Method
tc	1266.35	K	Joback Method
tf	713.90	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.31	J/mol×K	1008.18	Joback Method
cpg	1113.77	J/mol×K	1051.21	Joback Method
cpg	1151.03	J/mol×K	1094.24	Joback Method
cpg	1191.63	J/mol×K	1137.27	Joback Method
cpg	1236.12	J/mol×K	1180.30	Joback Method
cpg	1285.03	J/mol×K	1223.33	Joback Method
cpg	1338.91	J/mol×K	1266.35	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume