Silphiperfol-5-en-3-yl acetate A

Inchi: InChI=1S/C17H26O2/c1-10-6-7-17-12(3)11(2)9-16(17,5)15(8-14(10)17)19-13(4)18/h9-10
InchiKey: RQWCNVVRSOKTKR-GQADKEIASA-N
Formula: C17H26O2
SMILES: CC(=O)OC1CC2C(C)CCC23C(C)C(C)=CC13C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	2.61	kJ/mol	Joback Method
hf	-417.16	kJ/mol	Joback Method
hfus	24.23	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.957		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1652.00		NIST Webbook
tb	684.02	K	Joback Method
tc	905.33	K	Joback Method
tf	448.65	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.81	J/mol×K	684.02	Joback Method
cpg	692.40	J/mol×K	720.90	Joback Method
cpg	713.15	J/mol×K	757.79	Joback Method
cpg	733.32	J/mol×K	794.67	Joback Method
cpg	753.18	J/mol×K	831.56	Joback Method
cpg	772.97	J/mol×K	868.44	Joback Method
cpg	792.96	J/mol×K	905.33	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=R411857&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume