3-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-2-(1-acetate, (4bs-trans)-

Other names: Podocarpa-8,11,13-trien-12-ol, 13-isopropyl-, acetate
Acetyl ferruginol
trans-ferruginyl acetate
3-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-2-(1-methylethyl)-, 3-acetate, (4bS,8aS)-
Ferruginol acetate

Inchi: InChI=1S/C22H32O2/c1-14(2)17-12-16-8-9-20-21(4,5)10-7-11-22(20,6)18(16)13-19(17)2

InchiKey: AZEPENWNEVUZPW-UHFFFAOYSA-N

Formula: C22H32O2

SMILES: CC(=O)Oc1cc2c(cc1C(C)C)CCC1C(C)(C)CCCC21C

Mol. weight [g/mol]: 328.49

CAS: 15340-79-1

Physical Properties

Property code	Value	Unit	Source
gf	60.13	kJ/mol	Joback Method
hf	-401.95	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.766		Crippen Method
mcvol	282.800	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	2357.00		NIST Webbook
tb	838.06	K	Joback Method
tc	1069.64	K	Joback Method
tf	531.24	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.36	J/mol×K	838.06	Joback Method
cpg	941.34	J/mol×K	876.66	Joback Method
cpg	965.27	J/mol×K	915.25	Joback Method

cpg	989.45	J/mol×K	953.85	Joback Method
cpg	1014.16	J/mol×K	992.44	Joback Method
cpg	1039.71	J/mol×K	1031.04	Joback Method
cpg	1066.37	J/mol×K	1069.64	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=C15340791&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