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

Other names:	Podocarpa-8,11,13-trien-13-ol, 14-isopropyl-, acetate
	Totaryl acetate
	Totarol acetate
	2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, 2-acetate, (4bS,8aS)-
	2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, acetate, (4bS,8aS)-
Inchi:	InChI=1S/C22H32O2/c1-14(2)20-16-8-11-19-21(4,5)12-7-13-22(19,6)17(16)9-10-18(20)2
InchiKey:	ORVBSFQTFRBNRP-UHFFFAOYSA-N
Formula:	C22H32O2
SMILES:	CC(=O)Oc1ccc2c(c1C(C)C)CCC1C(C)(C)CCCC21C
Mol. weight [g/mol]:	328.49
CAS:	15340-82-6

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	2417.00		NIST Webbook
rinpol	2437.00		NIST Webbook
rinpol	2417.00		NIST Webbook
rinpol	2437.00		NIST Webbook
rinpol	2417.00		NIST Webbook
rinpol	2437.00		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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C15340826&Units=SI

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