9(1H)-Phenanthrenone, 2,3,4,4a,10,10a-hexahydro-6-hydroxy-1,1,4a-trime (4aS-trans)-

Other names: Podocarpa-8,11,13-trien-7-one, 12-hydroxy-13-isopropyl-
Sugiol
(4aS,10aS)-6-Hydroxy-7-isopropyl-1,1,4a-trimethyl-2,3,4,4a,10,10a-hexahydrophenanthr

Inchi: InChI=1S/C20H28O2/c1-12(2)13-9-14-15(10-16(13)21)20(5)8-6-7-19(3,4)18(20)11-17(14

InchiKey: IPEHJNRNYPOFII-UHFFFAOYSA-N

Formula: C20H28O2

SMILES: CC(C)c1cc2c(cc1O)C1(C)CCCC(C)(C)C1CC2=O

Mol. weight [g/mol]: 300.44

CAS: 511-05-7

Physical Properties

Property code	Value	Unit	Source
gf	9.63	kJ/mol	Joback Method
hf	-419.41	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	78.15	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.186		Crippen Method
mcvol	254.620	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	2659.90		NIST Webbook
rinpol	2659.90		NIST Webbook
tb	859.47	K	Joback Method
tc	1111.68	K	Joback Method
tf	603.96	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.19	J/mol×K	859.47	Joback Method
cpg	871.90	J/mol×K	901.51	Joback Method
cpg	897.24	J/mol×K	943.54	Joback Method
cpg	923.61	J/mol×K	985.58	Joback Method

cpg	951.45	J/mol×K	1027.61	Joback Method
cpg	981.15	J/mol×K	1069.65	Joback Method
cpg	1013.13	J/mol×K	1111.68	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=C511057&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