

1-Phenanthrenemethanol, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methyl-2-propenyl)-

Other names: Podocarpa-8,11,13-trien-15-ol, 10-isopropyl-7-abietyl alcohol, dehydro-

Dehydroabeityl alcohol
Dehydroabietinol
Dehydroabietol
[1R-(1«alpha»,4a«beta»,10a«alpha»)]-1,2,3,4,4a,9,10,10a-octahydro-7-isopropyl-1,4a-dimethyl-1-phenanthrenemethanol

Inchi: InChI=1S/C20H30O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/1-2,3,4,4a,9,10,10a

InchiKey: WSKGRAGZAQRSED-IOJLRTSASA-N

Formula: C20H30O

SMILES: CC(C)c1ccc2c(c1)CCC1C(C)(CO)CCCC21C

Mol. weight [g/mol]: 286.45

CAS: 3772-55-2

Physical Properties

Property code	Value	Unit	Source
gf	150.02	kJ/mol	Joback Method
hf	-256.63	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	77.56	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.813		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2354.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2378.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2386.60		NIST Webbook
rinpol	2386.60		NIST Webbook
ripol	3100.00		NIST Webbook
ripol	3100.00		NIST Webbook
tb	803.21	K	Joback Method
tc	1023.32	K	Joback Method
tf	484.84	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.48	J/mol×K	803.21	Joback Method
cpg	834.78	J/mol×K	839.89	Joback Method
cpg	855.97	J/mol×K	876.58	Joback Method
cpg	877.34	J/mol×K	913.26	Joback Method
cpg	899.15	J/mol×K	949.95	Joback Method
cpg	921.66	J/mol×K	986.63	Joback Method
cpg	945.17	J/mol×K	1023.32	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3772552&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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