

1-Naphthalenepropanol, «alpha»-ethenyldecahydro-4-hydroxy-«alpha»,5,5 [1S-[1«alpha»(R*),4«beta»,4a«beta»,8a«alpha»]]-

Other names:

Labdrol (20), 14-dien-6«alpha»,13-diol (13S)-
Larixol

Inchi: 1-Naphthalenepropanol,
«alpha»-ethenyldecahydro-4-hydroxy-«alpha»,5,5,8a-tetramethyl-2-methylene-
[1S-[1«alpha»(R*),4«beta»,4a«beta»,8a«alpha»]]-1,3-16(21)17-18(3,4)10-8-11-20(15,17)6

InchiKey: CLGDBTZPPRVUII-UHFFFAOYSA-N

Formula: C20H34O2

SMILES: C=CC(C)(O)CCC1C(=C)CC(O)C2C(C)(C)CCCC12C

Mol. weight [g/mol]: 306.48

CAS: 1438-66-0

Physical Properties

Property code	Value	Unit	Source
gf	26.63	kJ/mol	Joback Method
hf	-469.25	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	88.95	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.473		Crippen Method
mcvol	274.080	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2258.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2238.00		NIST Webbook
rinpol	2265.00		NIST Webbook
ripol	3270.00		NIST Webbook
ripol	3266.00		NIST Webbook
tb	851.00	K	Joback Method
tc	1054.41	K	Joback Method
tf	508.02	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.83	J/molxK	851.00	Joback Method
cpg	957.92	J/molxK	884.90	Joback Method
cpg	979.01	J/molxK	918.80	Joback Method
cpg	1000.30	J/molxK	952.71	Joback Method
cpg	1022.02	J/molxK	986.61	Joback Method
cpg	1044.37	J/molxK	1020.51	Joback Method
cpg	1067.56	J/molxK	1054.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1438660&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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