

1-Naphthalenepropanol, «alpha»-ethenyldecahydro-2-hydroxy-«alpha»,2,5 [1R-[1«alpha»(R*),2«beta»,4a«beta»,8a«alpha»]]-

Other names: 1-ahd-1,8,8,4,8-diol, (13R)-Sclareol
[1R-[1«alpha»(R*),2«beta»,4a«beta»,8a«alpha»]]-2-hydroxy-«alpha»,2,5,5,8a-pentamethyl-1,8-dihydro-1,4-methanonaphthalene
Inchi: InChI=1S/C20H36O2/c1-7-18(4,21)13-9-16-19(5)12-8-11-17(2,3)15(19)10-14-20(16,6)22
InchiKey: XVULBTBTFGYVRC-RBVQMXHFSA-N
Formula: C20H36O2
SMILES: C=CC(C)(O)CCC1C(C)(O)CCC2C(C)(C)CCCC21C
Mol. weight [g/mol]: 308.50
CAS: 515-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-31.94	kJ/mol	Joback Method
hf	-538.25	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.697		Crippen Method
mcvol	278.380	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	2247.00		NIST Webbook
rinpol	2229.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2225.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2225.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2238.70		NIST Webbook
tb	852.08	K	Joback Method

tc	1058.33	K	Joback Method
tf	518.24	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.67	J/mol×K	852.08	Joback Method
cpg	986.26	J/mol×K	886.45	Joback Method
cpg	1010.44	J/mol×K	920.83	Joback Method
cpg	1035.51	J/mol×K	955.20	Joback Method
cpg	1061.76	J/mol×K	989.58	Joback Method
cpg	1089.50	J/mol×K	1023.95	Joback Method
cpg	1119.02	J/mol×K	1058.33	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=C515037&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

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