1-Naphthalenemethanol, decahydro-5-(5-hydroxy-3-methyl-3-pentenyl)-1,4a-[1S-[1«alpha»,4a«alpha»,5«alpha»(E),8a«beta»]]-

Other names: Labda-8(20),13-diene-15,19-diol, (E)-
(+)-Agathadiol
Agathadienediol
Agathadiol
Agathadiol, (+)-
Contortadiol
Agatadiol

Inchi: InChI=1S/C20H34O2/c1-15(10-13-21)6-8-17-16(2)7-9-18-19(3,14-22)11-5-12-20(17,18)4

InchiKey: MJHWZTRFACWHTA-XNTDXEJSSA-N

Formula: C20H34O2

SMILES: C=C1CCC2C(C)(CO)CCCC2(C)C1CCC(C)=CCO

Mol. weight [g/mol]: 306.48

CAS: 1857-24-5

Physical Properties

Property code	Value	Unit	Source
gf	15.33	kJ/mol	Joback Method
hf	-458.16	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.476		Crippen Method
mcvol	274.080	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2266.00		NIST Webbook
tb	866.26	K	Joback Method
tc	1069.65	K	Joback Method
tf	492.56	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.70	J/mol×K	866.26	Joback Method

cpg	955.99	J/mol×K	900.16	Joback Method
cpg	977.42	J/mol×K	934.06	Joback Method
cpg	999.20	J/mol×K	967.96	Joback Method
cpg	1021.53	J/mol×K	1001.86	Joback Method
cpg	1044.64	J/mol×K	1035.75	Joback Method
cpg	1068.71	J/mol×K	1069.65	Joback Method

Sources

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=C1857245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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