Bicyclo[3.1.1]hept-2-ene-2-ethanol, 6,6-dimethyl-

Other names: 2-Norpinene-2-ethanol, 6,6-dimethyl-
Homomyrtenol
Nopol
Nopol (terpene)
6,6-Dimethyl-2-norpinene-2-ethanol
6,6-Dimethylbicyclo-(3,1,1)-heptene-2-ethanol
6,6-Dimethyl-2-(2-hydroxyethyl)-2-norpinene
6,6-Dimethylbicyclo-(3.1.1)-2-heptene-2-ethanol
Homomyretenol
Ethanol, 2(6,6-dimethyl-2-bicyclo[3.1.1] heptenyl)-
NSC 1284

Inchi: InChI=1S/C11H18O/c1-11(2)9-4-3-8(5-6-12)10(11)7-9/h3,9-10,12H,4-7H2,1-2H3

InchiKey: ROKSAUSPJGWCSM-UHFFFAOYSA-N

Formula: C11H18O

SMILES: CC1(C)C2CC=C(CCO)C1C2

Mol. weight [g/mol]: 166.26

CAS: 128-50-7

Physical Properties

Property code	Value	Unit	Source
gf	21.45	kJ/mol	Joback Method
hf	-241.95	kJ/mol	Joback Method
hfus	18.11	kJ/mol	Joback Method
hvap	56.25	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.361		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1212.00		NIST Webbook
ripol	1827.00		NIST Webbook
tb	560.72	K	Joback Method
tc	754.46	K	Joback Method
tf	339.85	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.10	J/mol×K	560.72	Joback Method
cpg	397.97	J/mol×K	593.01	Joback Method
cpg	411.95	J/mol×K	625.30	Joback Method
cpg	425.16	J/mol×K	657.59	Joback Method
cpg	437.71	J/mol×K	689.88	Joback Method
cpg	449.72	J/mol×K	722.17	Joback Method
cpg	461.28	J/mol×K	754.46	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=C128507&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume