(E)-2-((8R,8aS)-8,8a-Dimethyl-3,4,6,7,8,8a-hexahyd

Other names:	1-Propanol, 2-[(8R,8aS)-3,4,6,7,8,8a-hexahydro-8,8a-dimethyl-2(1H)-naphthalenylidene]-, (2E)-
	1-Propanol, 2-(3,4,6,7,8,8a-hexahydro-8,8a-dimethyl-2(1H)-naphthalenylidene)-, [8R-(2E,8«alpha»,8a«alpha»)]-
	4«beta»H,5«alpha»-Eremophila-1(10),7(11)-dien-12-ol
	(+)-Isovalencenol
	Isovalencenol
	(E)-Isovalencenol
	(E)-Eremophila-1(10),7(11)-dien-12-ol
Inchi:	InChI=1S/C15H24O/c1-11(10-16)13-7-8-14-6-4-5-12(2)15(14,3)9-13/h6,12,16H,4-5,7-10
InchiKey:	FXWSXJNUPFBCMQ-NVXNZCMISA-N
Formula:	C15H24O
SMILES:	CC(CO)=C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]:	220.35
CAS:	22387-74-2

Physical Properties

Property code	Value	Unit	Source
gf	63.45	kJ/mol	Joback Method
hf	-256.41	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.842		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	676.24	K	Joback Method
tc	886.47	K	Joback Method
tf	375.01	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.61	J/mol×K	676.24	Joback Method
cpg	588.71	J/mol×K	711.28	Joback Method
cpg	605.93	J/mol×K	746.32	Joback Method
cpg	622.42	J/mol×K	781.36	Joback Method
cpg	638.30	J/mol×K	816.40	Joback Method
cpg	653.73	J/mol×K	851.43	Joback Method
cpg	668.83	J/mol×K	886.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22387742&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

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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