(2R,3R,3aR,6R,8aS)-3,7,7-Trimethyl-8-methyleneo

Other names:	Zizanol
	2-epi-Ziza-6(13)-en-3«alpha»-ol
	1H-3a,6-Methanoazulen-2-ol, octahydro-3,7,7-trimethyl-8-methylene-, (2R,3R,3aR,6R,8aS)-
	1H-3a,6-Methanoazulen-2-ol, octahydro-3,7,7-trimethyl-8-methylene-, (2R,3S,3aR,6R,8aS)-(+)-
	1H-3a,6-Methanoazulen-2-ol, octahydro-3,7,7-trimethyl-8-methylene-, [2R-(2«alpha»,3«beta»,3a«beta»,6«beta»,8a«beta»)]-
	Ziza-6(13)-en-3«alpha»-ol
	2-epi-Ziza-6(13)-en-3-ol
Inchi:	InChI=1S/C15H24O/c1-9-12-7-13(16)10(2)15(12)6-5-11(8-15)14(9,3)4/h10-13,16H,1,5-8
InchiKey:	JZLOTPMXLYBVOH-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C1C2CC(O)C(C)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	220.35
CAS:	28102-79-6

Physical Properties

Property code	Value	Unit	Source
gf	115.62	kJ/mol	Joback Method
hf	-245.38	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	62.68	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1677.00		NIST Webbook
tb	649.17	K	Joback Method
tc	856.86	K	Joback Method
tf	415.17	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.53	J/mol×K	649.17	Joback Method

cpg	594.60	J/mol×K	683.79	Joback Method
cpg	612.82	J/mol×K	718.40	Joback Method
cpg	630.40	J/mol×K	753.02	Joback Method
cpg	647.59	J/mol×K	787.63	Joback Method
cpg	664.58	J/mol×K	822.25	Joback Method
cpg	681.62	J/mol×K	856.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28102796&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume