7-epi-cis-Dracunculifoliol

Inchi: InChI=1S/C15H26O/c1-10(2)14(16)12-7-9-15(4)8-5-6-11(3)13(12)15/h10,12-14,16H,3,5-
InchiKey: HKWKGGMAKOLVEY-CBBWQLFWSA-N
Formula: C15H26O
SMILES: C=C1CCCC2(C)CCC(C(O)C(C)C)C12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	58.80	kJ/mol	Joback Method
hf	-309.46	kJ/mol	Joback Method
hfus	15.23	kJ/mol	Joback Method
hvap	63.93	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1532.00		NIST Webbook
rinpol	1535.00		NIST Webbook
ripol	2015.00		NIST Webbook
tb	654.92	K	Joback Method
tc	856.87	K	Joback Method
tf	348.29	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.87	J/mol×K	654.92	Joback Method
cpg	612.12	J/mol×K	688.58	Joback Method
cpg	630.40	J/mol×K	722.24	Joback Method
cpg	647.83	J/mol×K	755.89	Joback Method
cpg	664.52	J/mol×K	789.55	Joback Method
cpg	680.61	J/mol×K	823.21	Joback Method
cpg	696.20	J/mol×K	856.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198866&Units=SI

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

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