cis-Dracunculifoliol

Inchi: InChI=1S/C16H28O/c1-11(2)14(17)16(5)10-9-15(4)8-6-7-12(3)13(15)16/h11,13-14,17H,3
InchiKey: XOCDJJVJLDUYLX-QKPAOTATSA-N
Formula: C16H28O
SMILES: C=C1CCCC2(C)CCC(C)(C(O)C(C)C)C12
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	61.73	kJ/mol	Joback Method
hf	-314.86	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.166		Crippen Method
mcvol	216.150	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1552.00		NIST Webbook
tb	678.04	K	Joback Method
tc	883.93	K	Joback Method
tf	383.46	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.39	J/mol×K	678.04	Joback Method
cpg	664.00	J/mol×K	712.35	Joback Method
cpg	682.87	J/mol×K	746.67	Joback Method
cpg	701.20	J/mol×K	780.98	Joback Method
cpg	719.19	J/mol×K	815.30	Joback Method
cpg	737.04	J/mol×K	849.61	Joback Method

cpg	754.96	J/mol×K	883.93	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=R418729&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume