(E)-dehydro-apofarnesol

Inchi: InChI=1S/C14H26O/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15/h7,9,14-15H,5-6,8,10-11H2,1
InchiKey: SVHDKVPXRARVAO-UKTHLTGXSA-N
Formula: C14H26O
SMILES: CC(C)=CCCC(C)=CCCC(C)CO
Mol. weight [g/mol]: 210.36

Physical Properties

Property code	Value	Unit	Source
gf	71.08	kJ/mol	Joback Method
hf	-274.94	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.088		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
tb	619.54	K	Joback Method
tc	794.30	K	Joback Method
tf	255.28	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.18	J/mol×K	619.54	Joback Method
cpg	557.74	J/mol×K	648.67	Joback Method
cpg	572.57	J/mol×K	677.79	Joback Method
cpg	586.71	J/mol×K	706.92	Joback Method
cpg	600.19	J/mol×K	736.05	Joback Method
cpg	613.06	J/mol×K	765.17	Joback Method
cpg	625.35	J/mol×K	794.30	Joback Method

Sources

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=R303612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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