Germacradienol

Inchi: InChI=1S/C15H26O/c1-12-6-5-7-13(2)9-11-14(10-8-12)15(3,4)16/h6,9,11,13-14,16H,5,7-
InchiKey: ZVZPKUXZGROCDB-FUMRZEMNSA-N
Formula: C15H26O
SMILES: CC1=CCCC(C)C=CC(C(C)(C)O)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-39.93	kJ/mol	Joback Method
hf	-400.48	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	66.42	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1549.00		NIST Webbook
rinpol	1583.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	666.81	K	Joback Method
tc	879.42	K	Joback Method
tf	325.15	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.99	J/mol×K	666.81	Joback Method
cpg	621.94	J/mol×K	702.24	Joback Method
cpg	641.52	J/mol×K	737.68	Joback Method
cpg	659.77	J/mol×K	773.11	Joback Method

cpg	676.70	J/mol×K	808.55	Joback Method
cpg	692.35	J/mol×K	843.98	Joback Method
cpg	706.73	J/mol×K	879.42	Joback Method
dvisc	0.0113104	Pa×s	325.15	Joback Method
dvisc	0.0016725	Pa×s	382.09	Joback Method
dvisc	0.0004061	Pa×s	439.04	Joback Method
dvisc	0.0001365	Pa×s	495.98	Joback Method
dvisc	0.0000574	Pa×s	552.92	Joback Method
dvisc	0.0000284	Pa×s	609.87	Joback Method
dvisc	0.0000158	Pa×s	666.81	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=R270007&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
dvisc:	Dynamic viscosity
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