4-«beta»-Hydro-germacra-1(10),5-diene

Inchi: InChI=1S/C15H26O/c1-11(2)14-8-5-12(3)6-10-15(16)13(4)7-9-14/h7,11,14-16H,3,5-6,8-1
InchiKey: SOEGJYPTWFJPTH-BYAULDSMSA-N
Formula: C15H26O
SMILES: C=C1CCC(O)C(C)=CCC(C(C)C)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-22.09	kJ/mol	Joback Method
hf	-370.55	kJ/mol	Joback Method
hfus	19.35	kJ/mol	Joback Method
hvap	67.20	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1570.90		NIST Webbook
tb	669.60	K	Joback Method
tc	875.08	K	Joback Method
tf	320.65	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.09	J/mol×K	669.60	Joback Method
cpg	618.60	J/mol×K	703.85	Joback Method
cpg	637.90	J/mol×K	738.09	Joback Method
cpg	655.97	J/mol×K	772.34	Joback Method
cpg	672.83	J/mol×K	806.59	Joback Method
cpg	688.46	J/mol×K	840.83	Joback Method
cpg	702.87	J/mol×K	875.08	Joback Method
dvisc	0.0107489	Pa×s	320.65	Joback Method
dvisc	0.0016524	Pa×s	378.81	Joback Method

dvisc	0.0004182	Pa×s	436.97	Joback Method
dvisc	0.0001461	Pa×s	495.12	Joback Method
dvisc	0.0000637	Pa×s	553.28	Joback Method
dvisc	0.0000325	Pa×s	611.44	Joback Method
dvisc	0.0000187	Pa×s	669.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R181096&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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