

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,3,5-6,8-10
InchiKey:	SOEGJYPTWFJPTH-BYAU LDSMSA-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
rinsol	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	m ³ /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	Paxs	320.65	Joback Method
dvisc	0.0016524	Paxs	378.81	Joback Method

dvisc	0.0004182	Paxs	436.97	Joback Method
dvisc	0.0001461	Paxs	495.12	Joback Method
dvisc	0.0000637	Paxs	553.28	Joback Method
dvisc	0.0000325	Paxs	611.44	Joback Method
dvisc	0.0000187	Paxs	669.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R181096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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