Guaia-3,10(14)-dien-11-ol

Inchi: InChI=1S/C15H24O/c1-10-5-7-12(15(3,4)16)9-14-11(2)6-8-13(10)14/h6,12-14,16H,1,5,7-
InchiKey: KOMASUWOXAIAJL-HZSPNIEDSA-N
Formula: C15H24O
SMILES: C=C1CCC(C(C)(C)O)CC2C(C)=CCC12
Mol. weight [g/mol]: 220.35
CAS: 176435-26-0

Physical Properties

Property code	Value	Unit	Source
gf	80.24	kJ/mol	Joback Method
hf	-282.74	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1672.00		NIST Webbook
tb	660.74	K	Joback Method
tc	867.43	K	Joback Method
tf	366.57	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.77	J/mol×K	660.74	Joback Method
cpg	596.79	J/mol×K	695.19	Joback Method
cpg	614.62	J/mol×K	729.64	Joback Method
cpg	631.32	J/mol×K	764.08	Joback Method
cpg	646.96	J/mol×K	798.53	Joback Method

cpg	661.60	J/mol×K	832.98	Joback Method
cpg	675.30	J/mol×K	867.43	Joback Method
dvisc	0.0040813	Pa×s	366.57	Joback Method
dvisc	0.0015755	Pa×s	415.60	Joback Method
dvisc	0.0007435	Pa×s	464.63	Joback Method
dvisc	0.0004050	Pa×s	513.65	Joback Method
dvisc	0.0002452	Pa×s	562.68	Joback Method
dvisc	0.0001609	Pa×s	611.71	Joback Method
dvisc	0.0001124	Pa×s	660.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C176435260&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
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
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