Guaia-1(10),11-dien-15-al

Inchi: InChI=1S/C15H22O/c1-10(2)12-5-6-13(9-16)14-7-4-11(3)15(14)8-12/h9,11-12,15H,1,4-8
InchiKey: BEDIGDJDGGJUFI-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC(C=O)=C2CCC(C)C2C1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	131.28	kJ/mol	Joback Method
hf	-187.41	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	622.83	K	Joback Method
tc	842.33	K	Joback Method
tf	328.45	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.43	J/mol×K	622.83	Joback Method
cpg	551.37	J/mol×K	659.41	Joback Method
cpg	571.01	J/mol×K	696.00	Joback Method
cpg	589.39	J/mol×K	732.58	Joback Method
cpg	606.58	J/mol×K	769.17	Joback Method
cpg	622.64	J/mol×K	805.75	Joback Method
cpg	637.60	J/mol×K	842.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R73189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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