

Guaia-1(10),11-dien-15,2-olide

Inchi:	InChI=1S/C15H20O2/c1-8-4-5-11-6-13-10(3)14(7-12(8)13)17-15(16)9(11)2/h9,11-12,14H
InchiKey:	WNLWOLXUWFZXOF-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	C=C1CCC2CC3=C(C)C(CC13)OC(=O)C2C
Mol. weight [g/mol]:	232.32

Physical Properties

Property code	Value	Unit	Source
gf	56.63	kJ/mol	Joback Method
hf	-330.13	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.241		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	678.28	K	Joback Method
tc	913.85	K	Joback Method
tf	428.58	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.96	J/mol×K	678.28	Joback Method
cpg	583.85	J/mol×K	717.54	Joback Method
cpg	603.34	J/mol×K	756.80	Joback Method
cpg	621.47	J/mol×K	796.06	Joback Method
cpg	638.29	J/mol×K	835.33	Joback Method
cpg	653.85	J/mol×K	874.59	Joback Method
cpg	668.18	J/mol×K	913.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R73175&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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