Guaia-1(10),11-dien-15-oic acid

Inchi: InChI=1S/C15H22O2/c1-9(2)11-5-7-13(15(16)17)12-6-4-10(3)14(12)8-11/h10-11,14H,1,4
InchiKey: JNYAUBXATZXFIU-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C(C)C1CCC(C(=O)O)=C2CCC(C)C2C1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-34.94	kJ/mol	Joback Method
hf	-366.64	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.790		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	720.22	K	Joback Method
tc	929.09	K	Joback Method
tf	397.20	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.62	J/mol×K	720.22	Joback Method
cpg	615.69	J/mol×K	755.03	Joback Method
cpg	631.67	J/mol×K	789.84	Joback Method
cpg	646.62	J/mol×K	824.65	Joback Method
cpg	660.58	J/mol×K	859.47	Joback Method
cpg	673.62	J/mol×K	894.28	Joback Method

cpg	685.76	J/mol×K	929.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613008&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
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