Guaja-1(10),11-dien-9-one

Inchi: InChI=1S/C15H22O/c1-9(2)12-6-5-10(3)15-13(8-12)11(4)7-14(15)16/h11-13H,1,5-8H2,2-
InchiKey: CKTOECQMCPFOEU-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC(C)=C2C(=O)CC(C)C2C1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	108.21	kJ/mol	Joback Method
hf	-239.53	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	54.46	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1752.00		NIST Webbook
tb	641.99	K	Joback Method
tc	871.82	K	Joback Method
tf	354.67	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.27	J/mol×K	641.99	Joback Method
cpg	565.40	J/mol×K	680.30	Joback Method
cpg	586.17	J/mol×K	718.60	Joback Method
cpg	605.60	J/mol×K	756.91	Joback Method
cpg	623.72	J/mol×K	795.21	Joback Method
cpg	640.55	J/mol×K	833.52	Joback Method
cpg	656.12	J/mol×K	871.82	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=R324946&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