

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

Inchi:	InChI=1S/C15H22O/c1-9(2)12-7-14-10(3)5-6-13(14)11(4)15(16)8-12/h10,12,14H,1,5-8H2
InchiKey:	YMXAKLYWISOQCM-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	<chem>C=C(C)C1CC(=O)C(C)=C2CCC(C)C2C1</chem>
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
hfus	20.91	kJ/mol	Joback Method
logp	3.904		Crippen Method
mcpvol	193.460	ml/mol	McGowan 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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613028&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/74-946-0/Guaia-1-10-11-dien-9-one.pdf>

Generated by Cheméo on 2026-07-22 20:18:19.018044734 +0000 UTC m=+262594.859930126.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.