

«alpha»-Guaiene

Other names:	Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1«alpha»,4«alpha»,7«alpha»)]- (1S,4S,7R)-1,4-Dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,5,6,7,8-octahydroazulene Guaia-1(5),11-diene 7-Isopropenyl-1,4-dimethyl-1,2,3,4,5,6,7,8-octahydroazulene-, [1S-(1«alpha»,4«alpha»,7«alpha»)]- Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, (1S,4S,7R)- «alpha»-Guajene «alpha»-quaiene «alpha»-Guaiaene
Inchi:	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h11-13H,1,5-9H2,2-4H3
InchiKey:	ADIDQIZBYUABQK-UPJWGTAASA-N
Formula:	C15H24
SMILES:	C=C(C)C1CCC(C)C2=C(C1)C(C)CC2
Mol. weight [g/mol]:	204.35
CAS:	3691-12-1

Physical Properties

Property code	Value	Unit	Source
gf	230.80	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1439.00		NIST Webbook

rinpol	1490.00	NIST Webbook
rinpol	1413.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1437.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1426.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1445.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1455.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1429.00	NIST Webbook
rinpol	1457.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1458.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1453.00	NIST Webbook

rinpol	1429.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1437.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1437.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1450.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1427.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1429.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1445.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1443.00	NIST Webbook
rinpol	1452.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1434.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1429.00	NIST Webbook
rinpol	1434.00	NIST Webbook
rinpol	1434.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1454.00	NIST Webbook

rinpol	1425.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1423.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1453.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1437.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1437.00	NIST Webbook
rinpol	1470.00	NIST Webbook
rinpol	1445.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1469.00	NIST Webbook
rinpol	1469.00	NIST Webbook
rinpol	1469.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1452.00	NIST Webbook
rinpol	1452.00	NIST Webbook
rinpol	1453.00	NIST Webbook
rinpol	1454.00	NIST Webbook
rinpol	1455.00	NIST Webbook
rinpol	1456.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1454.00	NIST Webbook
rinpol	1454.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1453.00	NIST Webbook
rinpol	1459.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1439.00	NIST Webbook

rinpol	1438.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1448.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1453.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1439.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1462.00	NIST Webbook
rinpol	1439.00	NIST Webbook
ripol	1652.00	NIST Webbook
ripol	1583.00	NIST Webbook
ripol	1596.00	NIST Webbook
ripol	1611.00	NIST Webbook
ripol	1596.00	NIST Webbook
ripol	1603.00	NIST Webbook
ripol	1578.00	NIST Webbook
ripol	1600.00	NIST Webbook

ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	574.17	K	Joback Method
tc	791.30	K	Joback Method
tf	286.45	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.80	J/mol×K	574.17	Joback Method
cpg	525.03	J/mol×K	610.36	Joback Method
cpg	546.90	J/mol×K	646.55	Joback Method
cpg	567.47	J/mol×K	682.74	Joback Method
cpg	586.78	J/mol×K	718.92	Joback Method
cpg	604.90	J/mol×K	755.11	Joback Method
cpg	621.88	J/mol×K	791.30	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=C3691121&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Latest version available from:

<https://www.chemeo.com/cid/21-366-2/alpha-Guaiene.pdf>

Generated by Cheméo on 2025-12-05 13:30:17.348792664 +0000 UTC m=+4689614.878833318.

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