Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methy
[1S-(1«alpha»,7«alpha»,8a«beta»)]-

Other names: (3S,3aS,7R)-3,8-Dimethyl-5-(prop-1-en-2-yl)-1,2,3,3a,4,5,6,7-octahydroazulene
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, (1S,7R,8aS)-
Guaia-1(10),11-diene
«alpha»-Bulnesene
«delta»-Guaiene
5-Isopropenyl-3,8-dimethyl-1,2,3,3a,4,5,6,7-octahydroazulene-, [1S-(1«alpha»,7«alpha»,8a«beta»)]-
«delta»-Guaiene («alpha»-bulnesene)
«delta»-Guaiene (= «alpha»-bulnesene)
«delta»-Guaijene

Inchi: InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h12-13,15H,1,5-9H2,2-4

InchiKey: YHAJBLWYOIUHHM-IKCIUXDWSA-N

Formula: C15H24

SMILES: C=C(C)C1CCC(C)=C2CCC(C)C2C1

Mol. weight [g/mol]: 204.35

CAS: 3691-11-0

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	1489.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1502.00		NIST Webbook

rinpol	1502.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1501.00	NIST Webbook
rinpol	1498.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1526.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1525.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1512.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1505.00	NIST Webbook

rinpol	1494.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1510.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1517.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1513.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1509.00	NIST Webbook
rinpol	1505.00	NIST Webbook
rinpol	1498.00	NIST Webbook
rinpol	1517.00	NIST Webbook
rinpol	1470.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1502.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1507.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1455.00	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1486.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1618.00	NIST Webbook
ripol	1613.00	NIST Webbook
ripol	1664.00	NIST Webbook
ripol	1629.00	NIST Webbook
ripol	1634.00	NIST Webbook

ripol	1642.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1613.00		NIST Webbook
tb	574.17	K	Joback Method
tc	791.30	K	Joback Method
tf	286.45	K	Joback Method
vc	0.725	m3/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=C3691110&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume