

«beta»-Guaiene

Other names:	Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethylidene)-, (1S-cis)-Guaia-1(5),7(11)-diene Guaiene 1,2,3,4,5,6,7,8-Octahydro-1,4-dimethyl-7-(1-methylethylidene)-azulene 1,4-Dimethyl-7-(1-methylethylidene)-1,2,3,4,5,6,7,8-octahydroazulene, (1S,cis)-«beta»-cis-Guaiene beta-Guaiene cis-«beta»-Guaiene «beta»-guainene cis-«beta»-Guainene (1S-cis)-1,2,3,4,5,6,7,8-octahydro-7-isopropylidene-1,4-dimethylazulene
Inchi:	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h11-12H,5-9H2,1-4H3/t1
InchiKey:	GIBQERSGRNPMEH-VXGBXAGGSA-N
Formula:	C15H24
SMILES:	<chem>CC(C)=C1CCC(C)C2=C(C1)C(C)CC2</chem>
Mol. weight [g/mol]:	204.35
CAS:	88-84-6

Physical Properties

Property code	Value	Unit	Source
gf	196.13	kJ/mol	Joback Method
hf	-130.89	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	51.98	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1489.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1490.00		NIST Webbook

rinpol	1490.00	NIST Webbook
rinpol	1469.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1479.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1499.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1487.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1462.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1486.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1481.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1487.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1485.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1462.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1487.00	NIST Webbook

rinpol	1490.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1529.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1481.00	NIST Webbook
rinpol	1467.00	NIST Webbook
rinpol	1458.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1489.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1486.00	NIST Webbook
rinpol	1513.00	NIST Webbook
rinpol	1462.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1478.00	NIST Webbook
rinpol	1465.00	NIST Webbook
rinpol	1451.00	NIST Webbook
rinpol	1451.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1478.00	NIST Webbook
rinpol	1491.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1488.00	NIST Webbook
rinpol	1478.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1504.00	NIST Webbook
rinpol	1482.00	NIST Webbook
rinpol	1476.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1495.00	NIST Webbook

ripol	1491.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1689.00		NIST Webbook
tb	588.80	K	Joback Method
tc	808.19	K	Joback Method
tf	302.81	K	Joback Method
vc	0.728	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.31	J/molxK	588.80	Joback Method
cpg	525.51	J/molxK	625.37	Joback Method
cpg	546.40	J/molxK	661.93	Joback Method
cpg	566.04	J/molxK	698.50	Joback Method
cpg	584.49	J/molxK	735.06	Joback Method
cpg	601.81	J/molxK	771.63	Joback Method
cpg	618.07	J/molxK	808.19	Joback Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C88846&Units=SI>

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

Latest version available from:

<https://www.cheméo.com/cid/63-609-6/beta-Guaiene.pdf>

Generated by Cheméo on 2024-05-02 01:41:33.993631268 +0000 UTC m=+16903342.914208580.

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