

1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1a«alpha»,4«alpha»,4a«beta»,7b«alpha»)]-

Other names:

1H-Cycloprop[e]azulene,
«alpha»-Gurjunene
1H-Cycloprop[e]azulene,
«alpha»-Gurjunene

(-)-«alpha»-Gurjunene

1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-,
(1a«alpha»,4«alpha»,4a«beta»,7b«alpha»)-
«alpha»-Gurgujene

«alpha»-Gurjenene

«alpha»-gurjinene

[1aR-(1a«alpha»,4«alpha»,4a«beta»,7b«alpha»)]-1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-

Inchi:	InChI=1S/C15H24/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h9,11-12,14H,5-8H2,1
InchiKey:	SPCXZDDGSGTVAW-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1=C2C(CC1)C(C)CCC1C2C1(C)C
Mol. weight [g/mol]:	204.35
CAS:	489-40-7

Physical Properties

Property code	Value	Unit	Source
gf	223.26	kJ/mol	Joback Method
hf	-137.45	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
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tb	571.38	K	Joback Method
tc	789.11	K	Joback Method
tf	346.81	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.59	J/mol×K	571.38	Joback Method
cpg	528.29	J/mol×K	607.67	Joback Method
cpg	549.58	J/mol×K	643.96	Joback Method
cpg	569.63	J/mol×K	680.24	Joback Method
cpg	588.60	J/mol×K	716.53	Joback Method
cpg	606.66	J/mol×K	752.82	Joback Method
cpg	624.00	J/mol×K	789.11	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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=C489407&Units=SI>

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

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