

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

Other names:

(+)-Ledene

1,1,4,7-Tetramethyl-1a,2,3,5,6,7,7a,7b-octahydro-1H-cyclopropa[e]azulene-,

[1aR-(1a«alpha»,7«alpha»,7a«beta»,7b«alpha»)]-

Viridiflorene

Leden

Ledene

(1aR,7R,7aS,7bR)-1,1,4,7-Tetramethyl-1a,2,3,5,6,7,7a,7b-octahydro-1H-cyclopropa[e]azulene

Viridiflorene

Viridiflorene

Viridiflorene (ledene)

[1aR-(1a«alpha»,7«alpha»,7a«beta»,7b«alpha»)]-1a,2,3,5,6,7,7a,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/h10,12-14H,5-8H2,1-4H
InchiKey:	WGTRJVCFDUCKCM-ZZVYKPCYSA-N
Formula:	C15H24
SMILES:	CC1=C2CCC(C)C2C2C(CC1)C2(C)C
Mol. weight [g/mol]:	204.35
CAS:	21747-46-6

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
rinpol	1486.00		NIST Webbook
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ripol	1688.00		NIST Webbook
ripol	1708.00		NIST Webbook
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

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=C21747466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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