

1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a«alpha»,4«beta»,4a«beta»,7«alpha»,7a«beta»,7b«alpha»)]-

Other names:

Viridiflorol

1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulen-4-ol-,

[1aR-(1a«alpha»,4«beta»,4a«beta»,7«alpha»,7a«beta»,7b«alpha»)]-

(+)-Viridiflorol

d-Viridiflorol

Himbaccol

Viridiflorol

Viridiflorol

[1aR-(1a«alpha»,4«beta»,4a«beta»,7«alpha»,7a«beta»,7b«alpha»)]-decahydro-1,1,4,7-

Inchi: InChI=1S/C15H26O/c1-9-5-6-10-12(9)13-11(14(13,2)3)7-8-15(10,4)16/h9-13,16H,5-8H2,

InchiKey: AYXPYQRXGNDJFU-JDBZYWECSA-N

Formula: C15H26O

SMILES: CC1CCC2C1C1C(CCC2(C)O)C1(C)C

Mol. weight [g/mol]: 222.37

CAS: 552-02-3

Physical Properties

Property code	Value	Unit	Source
gf	54.83	kJ/mol	Joback Method
hf	-349.96	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
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vc	0.742	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.58	J/mol×K	645.34	Joback Method
cpg	621.09	J/mol×K	679.69	Joback Method
cpg	640.66	J/mol×K	714.04	Joback Method
cpg	659.50	J/mol×K	748.38	Joback Method
cpg	677.83	J/mol×K	782.73	Joback Method
cpg	695.86	J/mol×K	817.08	Joback Method
cpg	713.82	J/mol×K	851.43	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C552023&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

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