

4,8-Methanoazulen-9-ol, decahydro-2,2,4,8-tetramethyl-, stereoisomer

Other names: 4,8-Methanoazulen-9-ol,
1,2,3,3a«alpha»,4,5,6,7,8,8a«alpha»-decahydro-2,2,4«beta»,8«beta»-tetramethyl-
«alpha»-Caryophyllene alcohol
11-Apollanol
«alpha»-Caryophyllenol

Inchi: InChI=1S/C15H26O/c1-13(2)8-10-11(9-13)15(4)7-5-6-14(10,3)12(15)16/h10-12,16H,5-9H

InchiKey: MJYUBUQHKCAJQR-UHFFFAOYSA-N

Formula: C15H26O

SMILES: CC1(C)CC2C(C1)C1(C)CCCC2(C)C1O

Mol. weight [g/mol]: 222.37

CAS: 4586-22-5

Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	425.39	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method
cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4586225&Units=SI
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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