

2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octah

Other names:	4,11-selinadiene
Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h13H,1,5-10H2,2-4H3
InchiKey:	MOTCYZHGM CNRH-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=C(C)C1CCC2(C)CCCC(C)=C2C1</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	233.02	kJ/mol	Joback Method
hf	-66.25	kJ/mol	Joback Method
hfus	14.03	kJ/mol	Joback Method
hvap	49.37	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1473.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1656.00		NIST Webbook
tb	579.08	K	Joback Method
tc	805.02	K	Joback Method
tf	314.59	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/molxK	579.08	Joback Method
cpg	522.29	J/molxK	616.74	Joback Method
cpg	543.51	J/molxK	654.39	Joback Method
cpg	563.48	J/molxK	692.05	Joback Method

cpg	582.36	J/mol×K	729.71	Joback Method
cpg	600.33	J/mol×K	767.36	Joback Method
cpg	617.54	J/mol×K	805.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U192435&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
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
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
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

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