

Dihydroisocaryophyllene

Inchi:	InChI=1S/C15H26/c1-11-6-5-7-14-13(10-15(14,3)4)12(2)9-8-11/h11,13-14H,2,5-10H2,1,3
InchiKey:	HIRBDDHEFKISPT-UHFFFAOYSA-N
Formula:	C15H26
SMILES:	C=C1CCC(C)CCCC2C1CC2(C)C
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	168.59	kJ/mol	Joback Method
hf	-179.33	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.805		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
ripol	1503.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1661.00		NIST Webbook
tb	567.49	K	Joback Method
tc	790.01	K	Joback Method
tf	306.19	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.19	J/molxK	567.49	Joback Method
cpg	546.68	J/molxK	604.58	Joback Method
cpg	570.65	J/molxK	641.66	Joback Method
cpg	593.23	J/molxK	678.75	Joback Method

cpg	614.55	J/mol×K	715.83	Joback Method
cpg	634.76	J/mol×K	752.92	Joback Method
cpg	653.96	J/mol×K	790.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R207742&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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