

Sativene

Inchi:	InChI=1S/C15H22/c1-9(2)11-7-13-12-5-6-14(13)15(4,8-11)10(12)3/h12-14H,3,5-8H2,1-2
InchiKey:	IDCAKVANYGLTQK-MLGYPOCJSA-N
Formula:	C15H22
SMILES:	<chem>C=C1C2CCC3C2CC(=C(C)C)CC13C</chem>
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	322.36	kJ/mol	Joback Method
hf	4.69	kJ/mol	Joback Method
hfus	19.54	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1437.00		NIST Webbook
rinpol	1396.00		NIST Webbook
tb	568.34	K	Joback Method
tc	787.10	K	Joback Method
tf	338.85	K	Joback Method
vc	0.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.37	J/mol×K	568.34	Joback Method
cpg	503.37	J/mol×K	604.80	Joback Method
cpg	522.95	J/mol×K	641.26	Joback Method
cpg	541.33	J/mol×K	677.72	Joback Method
cpg	558.69	J/mol×K	714.18	Joback Method
cpg	575.23	J/mol×K	750.64	Joback Method
cpg	591.15	J/mol×K	787.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R619135&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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