

Sativene

Other names:	(-)-sativene
Inchi:	InChI=1S/C15H24/c1-9(2)11-7-8-15(4)10(3)12-5-6-13(15)14(11)12/h9,11-14H,3,5-8H2,1
InchiKey:	VOBBUADSYROGAT-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=C1C2CCC3C2C(C(C)C)CCC13C</chem>
Mol. weight [g/mol]:	204.35
CAS:	6813-05-4

Physical Properties

Property code	Value	Unit	Source
gf	275.30	kJ/mol	Joback Method
hf	-87.17	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1394.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1387.00		NIST Webbook

ripol	1421.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1535.00		NIST Webbook
tb	556.71	K	Joback Method
tc	769.30	K	Joback Method
tf	323.21	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.63	J/molxK	556.71	Joback Method
cpg	524.39	J/molxK	592.14	Joback Method
cpg	545.67	J/molxK	627.57	Joback Method
cpg	565.65	J/molxK	663.00	Joback Method
cpg	584.49	J/molxK	698.44	Joback Method
cpg	602.37	J/molxK	733.87	Joback Method
cpg	619.46	J/molxK	769.30	Joback Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6813054&Units=SI>

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	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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