Isosativene

Other names: 2,4-Methano-1H-indene, octahydro-7a-methyl-1-methylene-5-(1-methylethyl)-, (2«alpha», 3a«beta», 4«alpha», 5«alpha», 7a«beta»)-
Inchi: InChI=1S/C15H24/c1-9(2)12-5-6-15(4)10(3)11-7-13(12)14(15)8-11/h9,11-14H,3,5-8H2,1-
InchiKey: CGZBLYYTRIVVTD-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C1C2CC3C(C(C)C)CCC1(C)C3C2
Mol. weight [g/mol]: 204.35
CAS: 24959-83-9

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	1452.00		NIST Webbook
rinpol	1417.60		NIST Webbook
rinpol	1417.60		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1454.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1676.00		NIST Webbook
tb	556.71	K	Joback Method
tc	769.30	K	Joback Method
tf	323.21	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24959839&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
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