

1H-Indene, 2,3,3a,4-tetrahydro-3,3a,6-trimethyl-1-(1-methylethyl)

Inchi:	InChI=1S/C15H24/c1-10(2)13-9-12(4)15(5)7-6-11(3)8-14(13)15/h6,8,10,12-13H,7,9H2,1-
InchiKey:	IVBZYUKCNLJUDA-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1=CCC2(C)C(=C1)C(C(C)C)CC2C
Mol. weight [g/mol]:	204.35
CAS:	59742-39-1

Physical Properties

Property code	Value	Unit	Source
gf	185.64	kJ/mol	Joback Method
hf	-143.57	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	49.39	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	572.30	K	Joback Method
tc	788.72	K	Joback Method
tf	315.35	K	Joback Method
vc	0.729	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.17	J/molxK	572.30	Joback Method
cpg	521.79	J/molxK	608.37	Joback Method
cpg	542.14	J/molxK	644.44	Joback Method
cpg	561.33	J/molxK	680.51	Joback Method
cpg	579.53	J/molxK	716.58	Joback Method
cpg	596.86	J/molxK	752.65	Joback Method
cpg	613.48	J/molxK	788.72	Joback Method

Sources

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=C59742391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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