

endo-1H-Indene, 3a,4,7,7a-tetrahydro, 4,7-ethano

Inchi:	InChI=1S/C11H14/c1-2-10-8-4-6-9(7-5-8)11(10)3-1/h1-2,4,6,8-11H,3,5,7H2/t8-,9+,10+,11-
InchiKey:	MOKDIRQGOJTXJX-VPLOUISSA-N
Formula:	C11H14
SMILES:	C1=CC2C3C=CC(CC3)C2C1
Mol. weight [g/mol]:	146.23

Physical Properties

Property code	Value	Unit	Source
gf	252.00	kJ/mol	Joback Method
hf	30.93	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	40.44	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.775		Crippen Method
mcvol	124.670	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinsol	1137.00		NIST Webbook
tb	473.49	K	Joback Method
tc	697.09	K	Joback Method
tf	257.79	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.58	J/molxK	473.49	Joback Method
cpg	375.02	J/molxK	659.82	Joback Method
cpg	360.13	J/molxK	622.56	Joback Method
cpg	344.05	J/molxK	585.29	Joback Method
cpg	326.67	J/molxK	548.02	Joback Method
cpg	307.88	J/molxK	510.76	Joback Method
cpg	388.81	J/molxK	697.09	Joback Method
dvisc	0.0010423	Paxs	473.49	Joback Method
dvisc	0.0010043	Paxs	437.54	Joback Method

dvisc	0.0009614	Paxs	401.59	Joback Method
dvisc	0.0009123	Paxs	365.64	Joback Method
dvisc	0.0008560	Paxs	329.69	Joback Method
dvisc	0.0007907	Paxs	293.74	Joback Method
dvisc	0.0007144	Paxs	257.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R128020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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