

1H-Indene, 2,3-dihydro-1,3-dimethyl-

Other names:	Indan, 1,3-dimethyl- 1,3-Dimethylindan 1,3-Dimethyl-(2,3-dihydroindene) 2,3-Dihydro-1,3-dimethyl-1H-indene
Inchi:	InChI=1S/C11H14/c1-8-7-9(2)11-6-4-3-5-10(8)11/h3-6,8-9H,7H2,1-2H3
InchiKey:	IIJUYSSJMAITHJ-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	CC1CC(C)c2ccccc21
Mol. weight [g/mol]:	146.23
CAS:	4175-53-5

Physical Properties

Property code	Value	Unit	Source
gf	197.56	kJ/mol	Joback Method
hf	7.15	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.297		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1127.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	200.61		NIST Webbook
tb	484.81	K	Joback Method
tc	704.37	K	Joback Method
tf	266.37	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	287.13	J/molxK	484.81	Joback Method
cpg	304.41	J/molxK	521.40	Joback Method
cpg	320.61	J/molxK	558.00	Joback Method
cpg	335.79	J/molxK	594.59	Joback Method
cpg	349.99	J/molxK	631.19	Joback Method
cpg	363.28	J/molxK	667.78	Joback Method
cpg	375.72	J/molxK	704.37	Joback Method
dvisc	0.0010979	Paxs	266.37	Joback Method
dvisc	0.0008508	Paxs	302.78	Joback Method
dvisc	0.0006964	Paxs	339.18	Joback Method
dvisc	0.0005926	Paxs	375.59	Joback Method
dvisc	0.0005189	Paxs	412.00	Joback Method
dvisc	0.0004642	Paxs	448.40	Joback Method
dvisc	0.0004223	Paxs	484.81	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=C4175535&Units=SI

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
mccvol:	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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