

1H-Indene, 1,3-dimethyl-

Other names:	(.+-.)-1,3-dimethyl-1H-indene
Inchi:	InChI=1S/C11H12/c1-8-7-9(2)11-6-4-3-5-10(8)11/h3-8H,1-2H3
InchiKey:	DZTYCPNBSJKSS-UHFFFAOYSA-N
Formula:	C11H12
SMILES:	CC1=CC(C)c2ccccc21
Mol. weight [g/mol]:	144.21
CAS:	2177-48-2

Physical Properties

Property code	Value	Unit	Source
gf	225.60	kJ/mol	Joback Method
hf	73.80	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	43.89	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.207		Crippen Method
mcvol	126.930	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	493.62	K	Joback Method
tc	716.95	K	Joback Method
tf	283.89	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.43	J/molxK	493.62	Joback Method
cpg	336.69	J/molxK	679.73	Joback Method
cpg	325.20	J/molxK	642.51	Joback Method
cpg	312.89	J/molxK	605.29	Joback Method
cpg	299.70	J/molxK	568.06	Joback Method
cpg	285.57	J/molxK	530.84	Joback Method
cpg	347.42	J/molxK	716.95	Joback Method
dvisc	0.0003923	Paxs	493.62	Joback Method

dvisc	0.0004348	Paxs	458.67	Joback Method
dvisc	0.0004900	Paxs	423.71	Joback Method
dvisc	0.0005644	Paxs	388.75	Joback Method
dvisc	0.0006684	Paxs	353.80	Joback Method
dvisc	0.0008214	Paxs	318.84	Joback Method
dvisc	0.0010621	Paxs	283.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2177482&Units=SI
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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