

1H-Indene, 1-methyl-

Other names:	1-METHYLINDENE 1-methyl-1(H)-indene ALPHA-METHYLINDENE Indene, 1-methyl- «alpha»-Methylindene Â«alphaÂ»-Methylindene
Inchi:	InChI=1S/C10H10/c1-8-6-7-9-4-2-3-5-10(8)9/h2-8H,1H3
InchiKey:	LRTOHSLOFCWHRF-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	CC1C=Cc2ccccc21
Mol. weight [g/mol]:	130.19
CAS:	767-59-9

Physical Properties

Property code	Value	Unit	Source
gf	226.81	kJ/mol	Joback Method
hf	105.91	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	41.00	kJ/mol	Joback Method
ie	8.27	eV	NIST Webbook
log10ws	-2.96		Crippen Method
logp	2.817		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	1172.00		NIST Webbook
rinpol	192.10		NIST Webbook
rinpol	193.84		NIST Webbook
rinpol	192.90		NIST Webbook
rinpol	192.10		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	193.40		NIST Webbook
rinpol	191.70		NIST Webbook
rinpol	1124.00		NIST Webbook
tb	465.76	K	Joback Method
tc	691.43	K	Joback Method
tf	260.10	K	Joback Method
vc	0.430	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.05	J/molxK	465.76	Joback Method
cpg	241.69	J/molxK	503.37	Joback Method
cpg	255.27	J/molxK	540.98	Joback Method
cpg	267.87	J/molxK	578.59	Joback Method
cpg	279.56	J/molxK	616.21	Joback Method
cpg	290.39	J/molxK	653.82	Joback Method
cpg	300.45	J/molxK	691.43	Joback Method
dvisc	0.0011190	Paxs	260.10	Joback Method
dvisc	0.0008468	Paxs	294.38	Joback Method
dvisc	0.0006792	Paxs	328.65	Joback Method
dvisc	0.0005679	Paxs	362.93	Joback Method
dvisc	0.0004898	Paxs	397.21	Joback Method
dvisc	0.0004324	Paxs	431.48	Joback Method
dvisc	0.0003889	Paxs	465.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.65394e+01
Coeff. B	-5.62766e+03
Coeff. C	-1.97000e+00
Temperature range (K), min.	348.25
Temperature range (K), max.	503.19

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.55331e+01
Coeff. B	-9.16109e+03
Coeff. C	-1.01485e+01
Coeff. D	4.38586e-06

Temperature range (K), min.	350.00
Temperature range (K), max.	703.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C767599&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=753
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=753

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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