3-METHYL-1H-INDENE

Other names:	1-Methyl-3H-indene
	3-Methylindene
	Indene, 3-methyl-
Inchi:	InChI=1S/C10H10/c1-8-6-7-9-4-2-3-5-10(8)9/h2-6H,7H2,1H3
InchiKey:	COOKKJGOGWACMY-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	CC1=CCc2ccccc21
Mol. weight [g/mol]:	130.19
CAS:	767-60-2

Physical Properties

Property code	Value	Unit	Source
hf	179.68	kJ/mol	Cheméo Relay (1.0)
hfus	13.21	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Cheméo Relay (1.0)
ie	8.05	eV	NIST Webbook
ie	7.97	eV	NIST Webbook
log10ws	-3.33		Cheméo Relay (1.0)
logp	2.646		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
rinpol	183.80		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	193.40		NIST Webbook
rinpol	184.10		NIST Webbook
rinpol	183.80		NIST Webbook
rinpol	1155.00		NIST Webbook
tb	486.09	K	Cheméo Relay (1.0)
tc	710.21	K	Cheméo Relay (1.0)
tf	246.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.56	J/mol×K	475.41	Joback Method

cpg	295.38	J/mol×K	702.69	Joback Method
cpg	285.94	J/mol×K	664.81	Joback Method
cpg	275.79	J/mol×K	626.93	Joback Method
cpg	264.84	J/mol×K	589.05	Joback Method
cpg	253.04	J/mol×K	551.17	Joback Method
cpg	240.30	J/mol×K	513.29	Joback Method
dvisc	0.0005835	Pa×s	376.13	Joback Method
dvisc	0.0003703	Pa×s	475.41	Joback Method
dvisc	0.0004212	Pa×s	442.32	Joback Method
dvisc	0.0004893	Pa×s	409.23	Joback Method
dvisc	0.0012738	Pa×s	276.86	Joback Method
dvisc	0.0007199	Pa×s	343.04	Joback Method
dvisc	0.0009289	Pa×s	309.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40784e+01
Coeff. B	-3.80216e+03
Coeff. C	-7.21300e+01
Temperature range (K), min.	347.83
Temperature range (K), max.	505.82

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C767602&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point