1H-INDENE, 2-METHYL-

Other names: 2-Methyl-1H-indene
2-methylindene
Indene, 2-methyl-
Inchi: InChI=1S/C10H10/c1-8-6-9-4-2-3-5-10(9)7-8/h2-6H,7H2,1H3
InchiKey: YSAXEHWHSLANOM-UHFFFAOYSA-N
Formula: C10H10
SMILES: CC1=Cc2ccccc2C1
Mol. weight [g/mol]: 130.19
CAS: 2177-47-1

Physical Properties

Property code	Value	Unit	Source
hfus	13.21	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	Cheméo Relay (1.0)
logp	2.646		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
rinpol	1054.10		NIST Webbook
rinpol	1057.70		NIST Webbook
rinpol	1057.70		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	184.40		NIST Webbook
rinpol	184.70		NIST Webbook
rinpol	192.61		NIST Webbook
rinpol	1054.10		NIST Webbook
tb	483.17	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.70	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46511e+01
Coeff. B	-4.00919e+03
Coeff. C	-7.44370e+01
Temperature range (K), min.	353.56
Temperature range (K), max.	503.70

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.50029e+01
Coeff. B	-8.85918e+03
Coeff. C	-1.01245e+01
Coeff. D	4.66607e-06
Temperature range (K), min.	353.15
Temperature range (K), max.	684.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=754
KDB:	https://www.cheric.org/files/research/kdb/mol/mol754.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2177471&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0, beta):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure