2-Methylindene

Other names: 1H-Indene, 2-methyl-
2-METHYL-1H-INDENE
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
gf	224.89	kJ/mol	Joback Method
hf	114.78	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.646		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	192.61		NIST Webbook
rinpol	184.40		NIST Webbook
rinpol	184.40		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1057.70		NIST Webbook
rinpol	1054.10		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1057.70		NIST Webbook
rinpol	184.70		NIST Webbook
rinpol	1054.10		NIST Webbook
tb	475.41	K	Joback Method
tc	702.69	K	Joback Method
tf	276.86	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.56	J/mol×K	475.41	Joback Method
cpg	240.30	J/mol×K	513.29	Joback Method
cpg	253.04	J/mol×K	551.17	Joback Method
cpg	264.84	J/mol×K	589.05	Joback Method
cpg	275.79	J/mol×K	626.93	Joback Method
cpg	285.94	J/mol×K	664.81	Joback Method
cpg	295.38	J/mol×K	702.69	Joback Method
dvisc	0.0012738	Pa×s	276.86	Joback Method
dvisc	0.0009289	Pa×s	309.95	Joback Method
dvisc	0.0007199	Pa×s	343.04	Joback Method
dvisc	0.0005835	Pa×s	376.13	Joback Method
dvisc	0.0004893	Pa×s	409.23	Joback Method
dvisc	0.0004212	Pa×s	442.32	Joback Method
dvisc	0.0003703	Pa×s	475.41	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

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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume