Isoprene

Other names:	1,3-Butadiene, 2-methyl-
	2-Methyl-1,3-butadiene
	2-Methylbuta-1,3-diene
	2-Methylbutadiene
	3-Methyl-1,3-butadiene
	CH2=C(CH3)CH=CH2
	Isopentadiene
	NSC 9237
	«beta»-Methylbivinyl
	Â«betaÂ»-Methylbivinyl
Inchi:	InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3
InchiKey:	RRHGJUQNOFWUDK-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	C=CC(=C)C
Mol. weight [g/mol]:	68.12
CAS:	78-79-5

Physical Properties

Property code	Value	Unit	Source
affp	826.40	kJ/mol	NIST Webbook
basg	797.60	kJ/mol	NIST Webbook
chg	-3186.60 ± 0.96	kJ/mol	NIST Webbook
chl	-3158.20 ± 1.60	kJ/mol	NIST Webbook
gf	158.35	kJ/mol	Joback Method
hf	75.70 ± 1.00	kJ/mol	NIST Webbook
hfus	4.84	kJ/mol	Joback Method
hvap	26.40	kJ/mol	NIST Webbook
hvap	26.80 ± 0.30	kJ/mol	NIST Webbook
ie	9.04	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.90 ± 0.10	eV	NIST Webbook
ie	8.85 ± 0.02	eV	NIST Webbook
ie	8.85 ± 0.01	eV	NIST Webbook
ie	8.84 ± 0.01	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.86 ± 0.02	eV	NIST Webbook
ie	8.87	eV	NIST Webbook

ie	8.85	eV	NIST Webbook
ie	8.89	eV	NIST Webbook
log10ws	-2.03		Estimated Solubility Method
log10ws	-2.03		Aqueous Solubility Prediction Method
logp	1.748		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	495.70		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	497.50		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	497.60		NIST Webbook
rinpol	491.50		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	497.00		NIST Webbook
rinpol	501.00		NIST Webbook
rinpol	501.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	504.00		NIST Webbook
rinpol	502.20		NIST Webbook
rinpol	504.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	497.00		NIST Webbook
rinpol	504.00		NIST Webbook
rinpol	505.00		NIST Webbook
rinpol	502.95		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	503.00		NIST Webbook
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rinpol	504.00		NIST Webbook
rinpol	503.00		NIST Webbook
rinpol	502.00		NIST Webbook
ripol	602.00		NIST Webbook
ripol	633.00		NIST Webbook
ripol	633.00		NIST Webbook
ripol	624.00		NIST Webbook
sg	314.76	J/mol×K	NIST Webbook
sl	229.20	J/mol×K	NIST Webbook
sl	229.30	J/mol×K	NIST Webbook
sl	228.28	J/mol×K	NIST Webbook
tb	307.20 ± 2.00	K	NIST Webbook
tb	307.00 ± 0.60	K	NIST Webbook
tb	307.20 ± 0.50	K	NIST Webbook
tb	307.30	K	NIST Webbook
tb	306.00 ± 2.00	K	NIST Webbook
tb	307.22 ± 0.20	K	NIST Webbook
tb	307.55 ± 1.50	K	NIST Webbook
tb	306.40 ± 1.00	K	NIST Webbook
tb	306.30 ± 1.00	K	NIST Webbook
tb	307.30 ± 0.50	K	NIST Webbook
tb	307.00 ± 1.50	K	NIST Webbook
tb	309.00 ± 2.00	K	NIST Webbook
tb	307.30 ± 0.50	K	NIST Webbook
tb	307.20 ± 1.00	K	NIST Webbook
tb	307.50 ± 0.50	K	NIST Webbook
tb	309.65 ± 1.00	K	NIST Webbook
tb	307.02 ± 0.60	K	NIST Webbook
tc	480.20	K	Joback Method
tf	127.18 ± 0.05	K	NIST Webbook
tf	153.00 ± 10.00	K	NIST Webbook
tf	127.01 ± 0.10	K	NIST Webbook
tf	127.18	K	Aqueous Solubility Prediction Method
tf	126.40 ± 0.40	K	NIST Webbook
tf	127.20 ± 0.03	K	NIST Webbook
tf	127.10 ± 0.40	K	NIST Webbook
tf	126.96 ± 0.20	K	NIST Webbook
tt	127.27 ± 0.05	K	NIST Webbook
tt	126.40 ± 0.20	K	NIST Webbook
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.42	J/mol×K	480.20	Joback Method
cpg	117.40	J/mol×K	364.76	Joback Method
cpg	124.63	J/mol×K	393.62	Joback Method
cpg	131.54	J/mol×K	422.48	Joback Method
cpg	138.13	J/mol×K	451.34	Joback Method
cpg	101.90	J/mol×K	307.04	Joback Method
cpg	109.82	J/mol×K	335.90	Joback Method
cpl	151.08	J/mol×K	298.15	NIST Webbook
cpl	152.60	J/mol×K	298.20	NIST Webbook
cpl	152.50	J/mol×K	298.15	NIST Webbook
hfust	4.92	kJ/mol	127.30	NIST Webbook
hfust	4.92	kJ/mol	127.30	NIST Webbook
hfust	4.83	kJ/mol	126.40	NIST Webbook
hfust	4.83	kJ/mol	126.40	NIST Webbook
hfust	4.92	kJ/mol	127.27	NIST Webbook
hvapt	31.50	kJ/mol	225.50	NIST Webbook
hvapt	28.30	kJ/mol	285.00	NIST Webbook
hvapt	29.40	kJ/mol	237.50	NIST Webbook
hvapt	25.80	kJ/mol	307.20	NIST Webbook
hvapt	27.40	kJ/mol	288.00	NIST Webbook
hvapt	27.30	kJ/mol	299.00	NIST Webbook
rfi	1.42180		293.15	Isobaric Vapor Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 250 kPa
sfust	38.21	J/mol×K	126.40	NIST Webbook
sfust	38.21	J/mol×K	126.40	NIST Webbook
sfust	38.69	J/mol×K	127.27	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	7.59285e+01
Coeff. B	-5.60831e+03
Coeff. C	-9.40749e+00
Coeff. D	8.78776e-06
Temperature range (K), min.	255.15
Temperature range (K), max.	483.30

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=365
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol365.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Isobaric Vapor Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 290 kPa:	https://www.doi.org/10.1021/acs.jced.6b00180
NISTWebbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78795&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume