1,3-Butadiene, 2,3-dimethyl-

Other names:	2,3-DIMETHYLENEBUTANE
	2,3-Dimethyl-1,3-butadiene
	2,3-Dimethylbuta-1,3-diene
	2,3-Dimethylbutadiene
	BIISOPROPENYL
	CH2=C(CH3)C(CH3)=CH2
	DIISOPROPENYL
Inchi:	InChI=1S/C6H10/c1-5(2)6(3)4/h1,3H2,2,4H3
InchiKey:	SDJHPPZKZZWAKF-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=C(C)C(=C)C
Mol. weight [g/mol]:	82.14
CAS:	513-81-5

Physical Properties

Property code	Value	Unit	Source
affp	835.00	kJ/mol	NIST Webbook
basg	807.80	kJ/mol	NIST Webbook
chl	-3815.00	kJ/mol	NIST Webbook
gf	158.22	kJ/mol	Joback Method
hf	64.11	kJ/mol	Joback Method
hfus	6.12	kJ/mol	Joback Method
hvap	31.00	kJ/mol	NIST Webbook
ie	8.54 ± 0.04	eV	NIST Webbook
ie	8.62	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
ie	8.66 ± 0.05	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.66	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.62 ± 0.02	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-2.40		Aqueous Solubility Prediction Method
log10ws	-2.40		Estimated Solubility Method

logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	612.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	598.30		NIST Webbook
rinpol	598.10		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	610.00		NIST Webbook
ripol	757.00		NIST Webbook
tb	338.00 ± 4.00	K	NIST Webbook
tb	342.00	K	NIST Webbook
tb	341.89 ± 0.40	K	NIST Webbook
tb	341.92 ± 0.40	K	NIST Webbook
tb	343.00 ± 2.00	K	NIST Webbook
tb	343.15 ± 2.00	K	NIST Webbook
tb	341.55	K	KDB
tb	344.15 ± 2.00	K	NIST Webbook
tb	340.70 ± 2.00	K	NIST Webbook
tb	343.00 ± 2.00	K	NIST Webbook
tb	342.00 ± 1.00	K	NIST Webbook
tb	341.50 ± 1.00	K	NIST Webbook
tb	342.90 ± 2.00	K	NIST Webbook
tb	342.15 ± 2.00	K	NIST Webbook
tc	507.31	K	Joback Method
tf	197.13	K	KDB
tf	197.13 ± 0.03	K	NIST Webbook
tf	197.14 ± 0.02	K	NIST Webbook
tf	197.20 ± 0.50	K	NIST Webbook

tf	208.00 ± 10.00	K	NIST Webbook
tf	196.89 ± 0.40	K	NIST Webbook
tf	197.12 ± 0.05	K	NIST Webbook
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.21	J/mol×K	329.80	Joback Method
cpg	142.84	J/mol×K	359.38	Joback Method
cpg	152.03	J/mol×K	388.97	Joback Method
cpg	160.82	J/mol×K	418.55	Joback Method
cpg	169.20	J/mol×K	448.14	Joback Method
cpg	177.19	J/mol×K	477.72	Joback Method
cpg	184.81	J/mol×K	507.31	Joback Method
hvapt	32.20	kJ/mol	307.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39098e+01
Coeff. B	-2.77268e+03
Coeff. C	-4.35880e+01
Temperature range (K), min.	247.13
Temperature range (K), max.	366.06

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.70887e+01
Coeff. B	-5.89288e+03
Coeff. C	-7.86671e+00
Coeff. D	5.66614e-06
Temperature range (K), min.	197.15
Temperature range (K), max.	526.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C513815&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=387
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol387.mol

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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