Butane, 1-iodo-3-methyl-

Other names:	1-Iodo-3-methylbutane
	1-Jod-3-methylbutan
	3-Methylbutyliodide
	4-Iodo-2-methylbutane
	CH2ICH2CH(CH3)2
	Isopentyl iodide
	iso-Amyliodide
	isoamyl iodide
Inchi:	InChI=1S/C5H11I/c1-5(2)3-4-6/h5H,3-4H2,1-2H3
InchiKey:	BUZZUHJODKQYTF-UHFFFAOYSA-N
Formula:	C5H11I
SMILES:	CC(C)CCI
Mol. weight [g/mol]:	198.05
CAS:	541-28-6

Physical Properties

Property code	Value	Unit	Source
gf	46.90	kJ/mol	Joback Method
hf	-74.94	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	42.20	kJ/mol	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
ie	9.17 ± 0.01	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.468		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	884.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1108.00		NIST Webbook
tb	420.80 ± 0.50	K	NIST Webbook
tb	420.80 ± 0.50	K	NIST Webbook
tb	420.80 ± 0.25	K	NIST Webbook
tb	419.00 ± 3.00	K	NIST Webbook

tb	420.80 ± 0.50	K	NIST Webbook
tc	613.94	K	Joback Method
tf	189.17	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.75	J/mol×K	613.94	Joback Method
cpg	182.14	J/mol×K	441.07	Joback Method
cpg	191.61	J/mol×K	475.65	Joback Method
cpg	200.59	J/mol×K	510.22	Joback Method
cpg	209.09	J/mol×K	544.79	Joback Method
cpg	217.13	J/mol×K	579.36	Joback Method
cpg	172.15	J/mol×K	406.50	Joback Method
cpl	178.70	J/mol×K	298.00	NIST Webbook
dvisc	0.0004932	Pa×s	370.28	Joback Method
dvisc	0.0010668	Pa×s	297.84	Joback Method
dvisc	0.0018416	Pa×s	261.61	Joback Method
dvisc	0.0037890	Pa×s	225.39	Joback Method
dvisc	0.0102765	Pa×s	189.17	Joback Method
dvisc	0.0003718	Pa×s	406.50	Joback Method
dvisc	0.0006956	Pa×s	334.06	Joback Method
hvapt	43.50	kJ/mol	346.00	NIST Webbook
pvap	0.13	kPa	269.10	Vapor Pressure of Selected Organic Iodides
pvap	0.18	kPa	273.61	Vapor Pressure of Selected Organic Iodides
pvap	0.18	kPa	273.61	Vapor Pressure of Selected Organic Iodides
pvap	0.25	kPa	278.56	Vapor Pressure of Selected Organic Iodides
pvap	0.25	kPa	278.57	Vapor Pressure of Selected Organic Iodides
pvap	0.25	kPa	278.58	Vapor Pressure of Selected Organic Iodides
pvap	0.13	kPa	268.98	Vapor Pressure of Selected Organic Iodides

pvap	0.35	kPa	283.55	Vapor Pressure of Selected Organic Iodides
pvap	0.35	kPa	283.56	Vapor Pressure of Selected Organic Iodides
pvap	0.48	kPa	288.52	Vapor Pressure of Selected Organic Iodides
pvap	0.48	kPa	288.53	Vapor Pressure of Selected Organic Iodides
pvap	0.48	kPa	288.54	Vapor Pressure of Selected Organic Iodides
pvap	0.66	kPa	293.55	Vapor Pressure of Selected Organic Iodides
pvap	0.66	kPa	293.55	Vapor Pressure of Selected Organic Iodides
pvap	0.66	kPa	293.57	Vapor Pressure of Selected Organic Iodides
pvap	0.87	kPa	298.43	Vapor Pressure of Selected Organic Iodides
pvap	0.88	kPa	298.44	Vapor Pressure of Selected Organic Iodides
pvap	0.88	kPa	298.44	Vapor Pressure of Selected Organic Iodides
pvap	1.16	kPa	303.29	Vapor Pressure of Selected Organic Iodides
pvap	1.16	kPa	303.29	Vapor Pressure of Selected Organic Iodides
pvap	1.16	kPa	303.29	Vapor Pressure of Selected Organic Iodides
pvap	0.06	kPa	258.62	Vapor Pressure of Selected Organic Iodides
pvap	0.06	kPa	258.62	Vapor Pressure of Selected Organic Iodides
pvap	0.04	kPa	253.70	Vapor Pressure of Selected Organic Iodides
pvap	0.04	kPa	253.68	Vapor Pressure of Selected Organic Iodides
pvap	0.04	kPa	253.67	Vapor Pressure of Selected Organic Iodides

pvap	0.18	kPa	273.61	Vapor Pressure of Selected Organic Iodides
pvap	0.35	kPa	283.55	Vapor Pressure of Selected Organic Iodides

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48981e+01
Coeff. B	-3.70808e+03
Coeff. C	-5.82850e+01
Temperature range (K), min.	312.08
Temperature range (K), max.	445.08

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541286&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressure of Selected Organic Iodides:	https://www.doi.org/10.1021/je100398m
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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

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