Butane, 1-iodo-

Other names:	1-Iodobutane
	1-Jodbutan
	Butyl iodide
	Iodobutane
	N-BUTYL IODIDE
	n-C4H9I
Inchi:	InChI=1S/C4H9I/c1-2-3-4-5/h2-4H2,1H3
InchiKey:	KMGBZBJJOKUPIA-UHFFFAOYSA-N
Formula:	C4H9I
SMILES:	CCCCI
Mol. weight [g/mol]:	184.02
CAS:	542-69-8

Physical Properties

Property code	Value	Unit	Source
gf	40.92	kJ/mol	Joback Method
hf	-49.02	kJ/mol	Joback Method
hfus	10.52	kJ/mol	Joback Method
hvap	40.60 ± 0.10	kJ/mol	NIST Webbook
hvap	40.63 ± 0.04	kJ/mol	NIST Webbook
hvap	35.40 ± 0.04	kJ/mol	NIST Webbook
hvap	40.67	kJ/mol	NIST Webbook
hvap	40.30	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.23 ± 0.01	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.24	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.23 ± 0.01	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.21 ± 0.01	eV	NIST Webbook
log10ws	-2.96		Aqueous Solubility Prediction Method

log10ws	-2.96		Estimated Solubility Method
logp	2.221		Crippen Method
mcvol	93.040	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	806.20		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	806.20		NIST Webbook
rinpol	819.30		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	844.90		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	806.00		NIST Webbook
ripol	1062.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1066.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1111.00		NIST Webbook
ripol	1062.00		NIST Webbook

ripol	1067.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1065.00		NIST Webbook
tb	403.55 ± 0.40	K	NIST Webbook
tb	403.70	K	NIST Webbook
tb	403.15 ± 4.00	K	NIST Webbook
tb	403.55 ± 0.50	K	NIST Webbook
tb	403.55	K	KDB
tb	399.00 ± 4.00	K	NIST Webbook
tb	403.70 ± 0.50	K	NIST Webbook
tb	403.85 ± 0.30	K	NIST Webbook
tb	403.05 ± 0.50	K	NIST Webbook
tb	403.70	K	NIST Webbook
tb	404.00 ± 2.00	K	NIST Webbook
tc	588.27	K	Joback Method
tf	169.65 ± 0.30	K	NIST Webbook
tf	143.15	K	KDB
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.06	J/mol×K	384.06	Joback Method
cpg	145.19	J/mol×K	418.10	Joback Method
cpg	152.91	J/mol×K	452.13	Joback Method
cpg	160.23	J/mol×K	486.17	Joback Method
cpg	167.16	J/mol×K	520.20	Joback Method
cpg	173.74	J/mol×K	554.24	Joback Method
cpg	179.97	J/mol×K	588.27	Joback Method
cpl	164.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0059605	Pa×s	192.90	Joback Method
dvisc	0.0027706	Pa×s	224.76	Joback Method
dvisc	0.0015577	Pa×s	256.62	Joback Method
dvisc	0.0009946	Pa×s	288.48	Joback Method
dvisc	0.0006943	Pa×s	320.34	Joback Method
dvisc	0.0004046	Pa×s	384.06	Joback Method
dvisc	0.0005172	Pa×s	352.20	Joback Method
hvapt	34.66	kJ/mol	403.70	NIST Webbook
hvapt	39.90	kJ/mol	361.50	NIST Webbook

rhol	1670.90	kg/m3	253.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1655.20	kg/m3	263.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1639.10	kg/m3	273.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1623.70	kg/m3	283.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1607.60	kg/m3	293.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1599.80	kg/m3	298.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1558.70	kg/m3	323.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K

rhol	1525.70	kg/m3	343.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1492.00	kg/m3	363.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1457.20	kg/m3	383.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46268e+01
Coeff. B	-3.58287e+03
Coeff. C	-4.50160e+01
Temperature range (K), min.	294.88
Temperature range (K), max.	429.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.36261e+01
Coeff. B	-7.91214e+03
Coeff. C	-1.18026e+01
Coeff. D	8.68183e-06
Temperature range (K), min.	292.15
Temperature range (K), max.	431.15

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (283.15 to 383.15) K:	https://www.doi.org/10.1021/je700020t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1611.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542698&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1611

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
rhol:	Liquid Density
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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