tert-Butyl iodide

Other names:	2-Iodo-2-methylpropane
	Propane, 2-iodo-2-methyl-
	Trimethyliodomethane
	tert-C4H9I
Inchi:	InChI=1S/C4H9I/c1-4(2,3)5/h1-3H3
InchiKey:	ANGGPYSFTXVERY-UHFFFAOYSA-N
Formula:	C4H9I
SMILES:	CC(C)(C)I
Mol. weight [g/mol]:	184.02
CAS:	558-17-8

Physical Properties

Property code	Value	Unit	Source
gf	43.76	kJ/mol	Joback Method
hf	-72.00 ± 1.00	kJ/mol	NIST Webbook
hfus	3.11	kJ/mol	Joback Method
hvap	35.50	kJ/mol	NIST Webbook
hvap	35.41 ± 0.06	kJ/mol	NIST Webbook
hvap	35.40 ± 0.10	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
ie	9.04	eV	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	9.09	eV	NIST Webbook
ie	9.02 ± 0.01	eV	NIST Webbook
ie	8.98 ± 0.01	eV	NIST Webbook
ie	9.02 ± 0.03	eV	NIST Webbook
log10ws	-2.56		Crippen Method
logp	2.220		Crippen Method
mcvol	93.040	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	698.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	699.00		NIST Webbook
tb	373.20	K	NIST Webbook
tb	372.00 ± 2.00	K	NIST Webbook

tb	373.20	K	NIST Webbook
tb	372.00	K	NIST Webbook
tc	599.98	K	Joback Method
tf	239.50 ± 0.30	K	NIST Webbook
vc	0.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.77	J/mol×K	380.83	Joback Method
cpg	148.37	J/mol×K	417.36	Joback Method
cpg	157.27	J/mol×K	453.88	Joback Method
cpg	165.51	J/mol×K	490.41	Joback Method
cpg	173.15	J/mol×K	526.93	Joback Method
cpg	180.21	J/mol×K	563.46	Joback Method
cpg	186.75	J/mol×K	599.98	Joback Method
dvisc	0.0023074	Pa×s	257.16	Joback Method
dvisc	0.0045630	Pa×s	226.24	Joback Method
dvisc	0.0111977	Pa×s	195.32	Joback Method
dvisc	0.0013507	Pa×s	288.07	Joback Method
dvisc	0.0008772	Pa×s	318.99	Joback Method
dvisc	0.0006148	Pa×s	349.91	Joback Method
dvisc	0.0004565	Pa×s	380.83	Joback Method
hsubt	49.80	kJ/mol	212.50	NIST Webbook
hvapt	31.43	kJ/mol	373.20	NIST Webbook
hvapt	34.80	kJ/mol	265.00	NIST Webbook
hvapt	33.10	kJ/mol	243.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35338e+01
Coeff. B	-2.76961e+03
Coeff. C	-6.25490e+01
Temperature range (K), min.	271.64
Temperature range (K), max.	399.39

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C558178&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume