Butane, 2-iodo-3-methyl-

Other names:	2-Iodo-3-methylbutane
	Butane, 3-methyl-2-iodo
Inchi:	InChI=1S/C5H11I/c1-4(2)5(3)6/h4-5H,1-3H3
InchiKey:	PYXUFKGRYMMOIK-UHFFFAOYSA-N
Formula:	C5H11I
SMILES:	CC(C)C(C)I
Mol. weight [g/mol]:	198.05
CAS:	18295-27-7

Physical Properties

Property code	Value	Unit	Source
gf	44.46	kJ/mol	Joback Method
hf	-80.22	kJ/mol	Joback Method
hfus	6.07	kJ/mol	Joback Method
hvap	35.32	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.466		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	941.00		NIST Webbook
ripol	1095.00		NIST Webbook
tb	406.06	K	Joback Method
tc	618.69	K	Joback Method
tf	174.17	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.18	J/mol×K	406.06	Joback Method
cpg	182.52	J/mol×K	441.50	Joback Method
cpg	192.31	J/mol×K	476.94	Joback Method
cpg	201.57	J/mol×K	512.37	Joback Method
cpg	210.33	J/mol×K	547.81	Joback Method

cpg	218.59	J/mol×K	583.25	Joback Method
cpg	226.40	J/mol×K	618.69	Joback Method
dvisc	0.0190621	Pa×s	174.17	Joback Method
dvisc	0.0053853	Pa×s	212.82	Joback Method
dvisc	0.0022438	Pa×s	251.47	Joback Method
dvisc	0.0011805	Pa×s	290.12	Joback Method
dvisc	0.0007223	Pa×s	328.76	Joback Method
dvisc	0.0004901	Pa×s	367.41	Joback Method
dvisc	0.0003580	Pa×s	406.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34862e+01
Coeff. B	-3.29325e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	305.52
Temperature range (K), max.	458.86

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18295277&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

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
hvap:	Enthalpy of vaporization at standard conditions
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