Butane, 2-iodo-2,3-dimethyl-

Other names: 2,3-Dimethyl-2-iodobutane
2-Iodo-2,3-dimethylbutane
Inchi: InChI=1S/C6H13I/c1-5(2)6(3,4)7/h5H,1-4H3
InchiKey: PRNFUXYRTWHXNG-UHFFFAOYSA-N
Formula: C6H13I
SMILES: CC(C)C(C)(C)I
Mol. weight [g/mol]: 212.07
CAS: 594-59-2

Physical Properties

Property code	Value	Unit	Source
gf	58.16	kJ/mol	Joback Method
hf	-104.33	kJ/mol	Joback Method
hfus	4.77	kJ/mol	Joback Method
hvap	36.64	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.856		Crippen Method
mcvol	121.220	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	426.15	K	Joback Method
tc	645.85	K	Joback Method
tf	202.86	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.03	J/mol×K	426.15	Joback Method
cpg	224.82	J/mol×K	462.77	Joback Method
cpg	236.75	J/mol×K	499.38	Joback Method
cpg	247.88	J/mol×K	536.00	Joback Method
cpg	258.24	J/mol×K	572.61	Joback Method
cpg	267.89	J/mol×K	609.23	Joback Method
cpg	276.89	J/mol×K	645.85	Joback Method

dvisc	0.0181053	Pa×s	202.86	Joback Method
dvisc	0.0057143	Pa×s	240.08	Joback Method
dvisc	0.0024579	Pa×s	277.29	Joback Method
dvisc	0.0012908	Pa×s	314.50	Joback Method
dvisc	0.0007769	Pa×s	351.72	Joback Method
dvisc	0.0005153	Pa×s	388.94	Joback Method
dvisc	0.0003672	Pa×s	426.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37723e+01
Coeff. B	-3.52652e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	323.92
Temperature range (K), max.	479.21

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=C594592&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume