2-Iodo-2-methylbutane

Other names: Butane, 2-iodo-2-methyl
Inchi: InChI=1S/C5H11I/c1-4-5(2,3)6/h4H2,1-3H3
InchiKey: NWRZTQFWFPLHHX-UHFFFAOYSA-N
Formula: C5H11I
SMILES: CCC(C)(C)I
Mol. weight [g/mol]: 198.05
CAS: 594-38-7

Physical Properties

Property code	Value	Unit	Source
gf	52.18	kJ/mol	Joback Method
hf	-78.41	kJ/mol	Joback Method
hfus	5.70	kJ/mol	Joback Method
hvap	34.80	kJ/mol	Joback Method
ie	8.93	eV	NIST Webbook
ie	8.93 ± 0.01	eV	NIST Webbook
log10ws	-2.98		Crippen Method
logp	2.610		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	829.00		NIST Webbook
rinpol	829.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1092.00		NIST Webbook
tb	397.70	K	NIST Webbook
tc	620.61	K	Joback Method
tf	206.59	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.17	J/mol×K	620.61	Joback Method
cpg	174.23	J/mol×K	403.71	Joback Method

cpg	185.30	J/mol×K	439.86	Joback Method
cpg	195.61	J/mol×K	476.01	Joback Method
cpg	205.21	J/mol×K	512.16	Joback Method
cpg	214.14	J/mol×K	548.31	Joback Method
cpg	222.44	J/mol×K	584.46	Joback Method
dvisc	0.0004201	Pa×s	403.71	Joback Method
dvisc	0.0108874	Pa×s	206.59	Joback Method
dvisc	0.0043620	Pa×s	239.44	Joback Method
dvisc	0.0021792	Pa×s	272.30	Joback Method
dvisc	0.0012642	Pa×s	305.15	Joback Method
dvisc	0.0008153	Pa×s	338.00	Joback Method
dvisc	0.0005683	Pa×s	370.86	Joback Method
hvapt	40.40	kJ/mol	353.00	NIST Webbook

Sources

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=C594387&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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
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