

Butane, 2-iodo-, (.+/-.)-

Inchi:	InChI=1S/C4H9I/c1-3-4(2)5/h4H,3H2,1-2H3
InchiKey:	IQRUSQUYPCHEKN-UHFFFAOYSA-N
Formula:	C4H9I
SMILES:	CCC(C)I
Mol. weight [g/mol]:	184.02
CAS:	52152-71-3

Physical Properties

Property code	Value	Unit	Source
gf	38.48	kJ/mol	Joback Method
hf	-54.30	kJ/mol	Joback Method
hfus	7.00	kJ/mol	Joback Method
hvap	33.48	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.220		Crippen Method
mcvol	93.040	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	393.20	K	NIST Webbook
tc	593.02	K	Joback Method
tf	177.90	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.04	J/molxK	383.62	Joback Method
cpg	175.01	J/molxK	558.12	Joback Method
cpg	168.23	J/molxK	523.22	Joback Method
cpg	161.06	J/molxK	488.32	Joback Method
cpg	153.49	J/molxK	453.42	Joback Method
cpg	145.49	J/molxK	418.52	Joback Method
cpg	181.41	J/molxK	593.02	Joback Method
dvisc	0.0003918	Paxs	383.62	Joback Method
dvisc	0.0005165	Paxs	349.33	Joback Method

dvisc	0.0007232	Paxs	315.05	Joback Method
dvisc	0.0010993	Paxs	280.76	Joback Method
dvisc	0.0018774	Paxs	246.47	Joback Method
dvisc	0.0038120	Paxs	212.19	Joback Method
dvisc	0.0101698	Paxs	177.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	306.20	K	6.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52152713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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