1-Butanol, 2-iodo-

Other names: 2-iodo-1-butanol
Inchi: InChI=1S/C4H9IO/c1-2-4(5)3-6/h4,6H,2-3H2,1H3
InchiKey: GVYHZUNZPGWEPZ-UHFFFAOYSA-N
Formula: C4H9IO
SMILES: CCC(I)CO
Mol. weight [g/mol]: 200.02
CAS: 127201-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-98.34	kJ/mol	Joback Method
hf	-206.53	kJ/mol	Joback Method
hfus	11.09	kJ/mol	Joback Method
hvap	50.16	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.192		Crippen Method
mcvol	98.910	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	475.80	K	Joback Method
tc	674.21	K	Joback Method
tf	238.72	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.03	J/mol×K	475.80	Joback Method
cpg	206.84	J/mol×K	641.14	Joback Method
cpg	200.99	J/mol×K	608.07	Joback Method
cpg	194.79	J/mol×K	575.00	Joback Method
cpg	188.25	J/mol×K	541.94	Joback Method
cpg	181.33	J/mol×K	508.87	Joback Method
cpg	212.39	J/mol×K	674.21	Joback Method
dvisc	0.0002665	Pa×s	475.80	Joback Method

dvisc	0.0004542	Pa×s	436.29	Joback Method
dvisc	0.0008606	Pa×s	396.77	Joback Method
dvisc	0.0018783	Pa×s	357.26	Joback Method
dvisc	0.0049775	Pa×s	317.75	Joback Method
dvisc	0.0173977	Pa×s	278.23	Joback Method
dvisc	0.0920207	Pa×s	238.72	Joback Method

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=C127201289&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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