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

Physical Properties

Property code	Value	Unit	Source
hf	-185.58	kJ/mol	Cheméo Relay (1.0)
hfus	11.09	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Cheméo Relay (1.0)
ie	9.35	eV	Cheméo Relay (1.0)
log10ws	-0.95		Cheméo Relay (1.0)
logp	1.192		Crippen Method
mcvol	98.910	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	463.97	K	Cheméo Relay (1.0)
tc	724.52	K	Cheméo Relay (1.0)
tf	240.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.03	J/mol×K	475.80	Joback Method
cpg	212.39	J/mol×K	674.21	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
dvisc	0.0018783	Pa×s	357.26	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	0.0920207	Pa×s	238.72	Joback Method
dvisc	0.0049775	Pa×s	317.75	Joback Method
dvisc	0.0173977	Pa×s	278.23	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127201289&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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