Butanoic acid, 3-methyl, 2-iodoethyl ester

Inchi: InChI=1S/C7H13IO2/c1-6(2)5-7(9)10-4-3-8/h6H,3-5H2,1-2H3
InchiKey: ANMUQHGRSUBSQJ-UHFFFAOYSA-N
Formula: C7H13IO2
SMILES: CC(C)CC(=O)OCCI
Mol. weight [g/mol]: 256.08

Physical Properties

Property code	Value	Unit	Source
gf	-170.18	kJ/mol	Joback Method
hf	-361.02	kJ/mol	Joback Method
hfus	17.56	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.011		Crippen Method
mcvol	142.750	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1203.00		NIST Webbook
tb	528.55	K	Joback Method
tc	739.58	K	Joback Method
tf	283.87	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.34	J/mol×K	528.55	Joback Method
cpg	299.75	J/mol×K	563.72	Joback Method
cpg	310.60	J/mol×K	598.89	Joback Method
cpg	320.88	J/mol×K	634.07	Joback Method
cpg	330.61	J/mol×K	669.24	Joback Method
cpg	339.81	J/mol×K	704.41	Joback Method
cpg	348.49	J/mol×K	739.58	Joback Method
dvisc	0.0046711	Pa×s	283.87	Joback Method
dvisc	0.0021715	Pa×s	324.65	Joback Method

dvisc	0.0011976	Pa×s	365.43	Joback Method
dvisc	0.0007444	Pa×s	406.21	Joback Method
dvisc	0.0005046	Pa×s	446.99	Joback Method
dvisc	0.0003650	Pa×s	487.77	Joback Method
dvisc	0.0002776	Pa×s	528.55	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R19854&Units=SI

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume