Propionic acid, 3-iodo-, butyl ester

Inchi: InChI=1S/C7H13IO2/c1-2-3-6-10-7(9)4-5-8/h2-6H2,1H3
InchiKey: GFBSJOIIEKBRHY-UHFFFAOYSA-N
Formula: C7H13IO2
SMILES: CCCCOC(=O)CCI
Mol. weight [g/mol]: 256.08

Physical Properties

Property code	Value	Unit	Source
gf	-167.74	kJ/mol	Joback Method
hf	-355.74	kJ/mol	Joback Method
hfus	21.08	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.155		Crippen Method
mcvol	142.750	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
tb	528.99	K	Joback Method
tc	735.45	K	Joback Method
tf	298.87	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.01	J/mol×K	528.99	Joback Method
cpg	299.10	J/mol×K	563.40	Joback Method
cpg	309.66	J/mol×K	597.81	Joback Method
cpg	319.70	J/mol×K	632.22	Joback Method
cpg	329.21	J/mol×K	666.63	Joback Method
cpg	338.23	J/mol×K	701.04	Joback Method
cpg	346.75	J/mol×K	735.45	Joback Method
dvisc	0.0034653	Pa×s	298.87	Joback Method

dvisc	0.0018193	Pa×s	337.22	Joback Method
dvisc	0.0010895	Pa×s	375.58	Joback Method
dvisc	0.0007175	Pa×s	413.93	Joback Method
dvisc	0.0005072	Pa×s	452.28	Joback Method
dvisc	0.0003785	Pa×s	490.64	Joback Method
dvisc	0.0002947	Pa×s	528.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406239&Units=SI
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

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