Propionic acid, 3-iodo-, propyl ester

Inchi: InChI=1S/C6H11IO2/c1-2-5-9-6(8)3-4-7/h2-5H2,1H3
InchiKey: CNTHQHNTVHYYJW-UHFFFAOYSA-N
Formula: C6H11IO2
SMILES: CCCOC(=O)CCI
Mol. weight [g/mol]: 242.05

Physical Properties

Property code	Value	Unit	Source
gf	-176.16	kJ/mol	Joback Method
hf	-335.10	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	47.48	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.765		Crippen Method
mcvol	128.660	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1216.00		NIST Webbook
tb	506.11	K	Joback Method
tc	715.74	K	Joback Method
tf	287.60	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.54	J/mol×K	506.11	Joback Method
cpg	255.51	J/mol×K	541.05	Joback Method
cpg	264.99	J/mol×K	575.99	Joback Method
cpg	274.01	J/mol×K	610.93	Joback Method
cpg	282.57	J/mol×K	645.86	Joback Method
cpg	290.68	J/mol×K	680.80	Joback Method
cpg	298.35	J/mol×K	715.74	Joback Method
dvisc	0.0035969	Pa×s	287.60	Joback Method

dvisc	0.0019254	Pa×s	324.02	Joback Method
dvisc	0.0011694	Pa×s	360.44	Joback Method
dvisc	0.0007783	Pa×s	396.86	Joback Method
dvisc	0.0005547	Pa×s	433.27	Joback Method
dvisc	0.0004167	Pa×s	469.69	Joback Method
dvisc	0.0003261	Pa×s	506.11	Joback Method

Sources

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=U406237&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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