Propanoic acid, 2-iodoethyl ester

Inchi: InChI=1S/C5H9IO2/c1-2-5(7)8-4-3-6/h2-4H2,1H3
InchiKey: YXIMMRXXZQYICY-UHFFFAOYSA-N
Formula: C5H9IO2
SMILES: CCC(=O)OCCI
Mol. weight [g/mol]: 228.03

Physical Properties

Property code	Value	Unit	Source
gf	-184.58	kJ/mol	Joback Method
hf	-314.46	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	45.25	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.375		Crippen Method
mcvol	114.570	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1063.00		NIST Webbook
tb	483.23	K	Joback Method
tc	696.06	K	Joback Method
tf	276.33	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.12	J/mol×K	483.23	Joback Method
cpg	244.50	J/mol×K	660.59	Joback Method
cpg	237.42	J/mol×K	625.12	Joback Method
cpg	229.94	J/mol×K	589.64	Joback Method
cpg	222.07	J/mol×K	554.17	Joback Method
cpg	213.80	J/mol×K	518.70	Joback Method
cpg	251.21	J/mol×K	696.06	Joback Method
dvisc	0.0003583	Pa×s	483.23	Joback Method
dvisc	0.0004552	Pa×s	448.75	Joback Method

dvisc	0.0006017	Pa×s	414.26	Joback Method
dvisc	0.0008369	Pa×s	379.78	Joback Method
dvisc	0.0012431	Pa×s	345.30	Joback Method
dvisc	0.0020161	Pa×s	310.81	Joback Method
dvisc	0.0036892	Pa×s	276.33	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=R20053&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

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