Hexanoic acid, 2-iodoethyl ester

Inchi: InChI=1S/C8H15IO2/c1-2-3-4-5-8(10)11-7-6-9/h2-7H2,1H3
InchiKey: FNQXKZGQRWXHAK-UHFFFAOYSA-N
Formula: C8H15IO2
SMILES: CCCCCC(=O)OCCI
Mol. weight [g/mol]: 270.11

Physical Properties

Property code	Value	Unit	Source
gf	-159.32	kJ/mol	Joback Method
hf	-376.38	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.545		Crippen Method
mcvol	156.840	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1384.00		NIST Webbook
tb	551.87	K	Joback Method
tc	755.24	K	Joback Method
tf	310.14	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.40	J/mol×K	551.87	Joback Method
cpg	387.10	J/mol×K	721.34	Joback Method
cpg	377.28	J/mol×K	687.45	Joback Method
cpg	366.92	J/mol×K	653.55	Joback Method
cpg	356.00	J/mol×K	619.66	Joback Method
cpg	344.49	J/mol×K	585.76	Joback Method
cpg	396.37	J/mol×K	755.24	Joback Method
dvisc	0.0002646	Pa×s	551.87	Joback Method

dvisc	0.0003415	Pa×s	511.58	Joback Method
dvisc	0.0004603	Pa×s	471.29	Joback Method
dvisc	0.0006562	Pa×s	431.00	Joback Method
dvisc	0.0010063	Pa×s	390.72	Joback Method
dvisc	0.0017028	Pa×s	350.43	Joback Method
dvisc	0.0033031	Pa×s	310.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R19779&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