Pentanoic acid, 4-methyl, 2-iodoethyl ester

Inchi: InChI=1S/C8H15IO2/c1-7(2)3-4-8(10)11-6-5-9/h7H,3-6H2,1-2H3
InchiKey: DWAAMYINEBPDQR-UHFFFAOYSA-N
Formula: C8H15IO2
SMILES: CC(C)CCC(=O)OCCI
Mol. weight [g/mol]: 270.11

Physical Properties

Property code	Value	Unit	Source
gf	-161.76	kJ/mol	Joback Method
hf	-381.66	kJ/mol	Joback Method
hfus	20.15	kJ/mol	Joback Method
hvap	51.54	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.401		Crippen Method
mcvol	156.840	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	551.43	K	Joback Method
tc	759.14	K	Joback Method
tf	295.14	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.76	J/mol×K	551.43	Joback Method
cpg	388.73	J/mol×K	724.52	Joback Method
cpg	378.73	J/mol×K	689.90	Joback Method
cpg	368.15	J/mol×K	655.29	Joback Method
cpg	356.97	J/mol×K	620.67	Joback Method
cpg	345.18	J/mol×K	586.05	Joback Method
cpg	398.16	J/mol×K	759.14	Joback Method
dvisc	0.0002485	Pa×s	551.43	Joback Method

dvisc	0.0003281	Pa×s	508.72	Joback Method
dvisc	0.0004559	Pa×s	466.00	Joback Method
dvisc	0.0006768	Pa×s	423.29	Joback Method
dvisc	0.0010982	Pa×s	380.57	Joback Method
dvisc	0.0020138	Pa×s	337.86	Joback Method
dvisc	0.0044013	Pa×s	295.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R20049&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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