Nonanoic acid, 2-iodoethyl ester

Inchi: InChI=1S/C11H21IO2/c1-2-3-4-5-6-7-8-11(13)14-10-9-12/h2-10H2,1H3
InchiKey: RLDJLWYTRGYSFO-UHFFFAOYSA-N
Formula: C11H21IO2
SMILES: CCCCCCCCC(=O)OCCI
Mol. weight [g/mol]: 312.19

Physical Properties

Property code	Value	Unit	Source
gf	-134.06	kJ/mol	Joback Method
hf	-438.30	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.715		Crippen Method
mcvol	199.110	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1683.00		NIST Webbook
tb	620.51	K	Joback Method
tc	815.62	K	Joback Method
tf	343.95	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.09	J/mol×K	620.51	Joback Method
cpg	541.13	J/mol×K	783.11	Joback Method
cpg	529.48	J/mol×K	750.59	Joback Method
cpg	517.16	J/mol×K	718.07	Joback Method
cpg	504.17	J/mol×K	685.55	Joback Method
cpg	490.49	J/mol×K	653.03	Joback Method
cpg	552.15	J/mol×K	815.62	Joback Method
dvisc	0.0001855	Pa×s	620.51	Joback Method
dvisc	0.0002424	Pa×s	574.42	Joback Method

dvisc	0.0003320	Pa×s	528.32	Joback Method
dvisc	0.0004827	Pa×s	482.23	Joback Method
dvisc	0.0007598	Pa×s	436.14	Joback Method
dvisc	0.0013314	Pa×s	390.04	Joback Method
dvisc	0.0027112	Pa×s	343.95	Joback Method

Sources

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=R19957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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