Nonanoic acid, 9,9-diethoxy-, ethyl ester

Other names: Ethyl 9,9-diethoxynonanoate
Inchi: InChI=1S/C15H30O4/c1-4-17-14(16)12-10-8-7-9-11-13-15(18-5-2)19-6-3/h15H,4-13H2,1
InchiKey: FUHCSXNXTVRKIW-UHFFFAOYSA-N
Formula: C15H30O4
SMILES: CCOC(=O)CCCCCCCC(OCC)OCC
Mol. weight [g/mol]: 274.40
CAS: 74987-89-6

Physical Properties

Property code	Value	Unit	Source
gf	-370.94	kJ/mol	Joback Method
hf	-867.45	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.679		Crippen Method
mcvol	241.390	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1765.70		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	663.29	K	Joback Method
tc	833.94	K	Joback Method
tf	360.43	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.61	J/mol×K	663.29	Joback Method
cpg	760.49	J/mol×K	805.49	Joback Method
cpg	746.20	J/mol×K	777.05	Joback Method
cpg	731.17	J/mol×K	748.61	Joback Method
cpg	715.39	J/mol×K	720.17	Joback Method
cpg	698.87	J/mol×K	691.73	Joback Method

cpg	774.04	J/mol×K	833.94	Joback Method
dvisc	0.0000765	Pa×s	663.29	Joback Method
dvisc	0.0001028	Pa×s	612.81	Joback Method
dvisc	0.0001455	Pa×s	562.34	Joback Method
dvisc	0.0002206	Pa×s	511.86	Joback Method
dvisc	0.0003664	Pa×s	461.38	Joback Method
dvisc	0.0006891	Pa×s	410.91	Joback Method
dvisc	0.0015473	Pa×s	360.43	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74987896&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

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