Nonanoic acid, 9-oxo-, ethyl ester

Other names: Ethyl 9-oxononanoate
Inchi: InChI=1S/C11H20O3/c1-2-14-11(13)9-7-5-3-4-6-8-10-12/h10H,2-9H2,1H3
InchiKey: RVICDIQCDUVBFK-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CCOC(=O)CCCCCCCC=O
Mol. weight [g/mol]: 200.27
CAS: 3433-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-291.70	kJ/mol	Joback Method
hf	-600.75	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.479		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	576.03	K	Joback Method
tc	751.60	K	Joback Method
tf	327.89	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.05	J/mol×K	576.03	Joback Method
cpg	452.84	J/mol×K	605.29	Joback Method
cpg	466.04	J/mol×K	634.55	Joback Method
cpg	478.67	J/mol×K	663.81	Joback Method

cpg	490.73	J/mol×K	693.08	Joback Method
cpg	502.23	J/mol×K	722.34	Joback Method
cpg	513.18	J/mol×K	751.60	Joback Method
dvisc	0.0028915	Pa×s	327.89	Joback Method
dvisc	0.0015073	Pa×s	369.25	Joback Method
dvisc	0.0008959	Pa×s	410.60	Joback Method
dvisc	0.0005857	Pa×s	451.96	Joback Method
dvisc	0.0004112	Pa×s	493.32	Joback Method
dvisc	0.0003049	Pa×s	534.67	Joback Method
dvisc	0.0002360	Pa×s	576.03	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=C3433167&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume