Nonanoic acid, 6-oxo-, ethyl ester

Other names: ethyl 6-oxononanoate
Inchi: InChI=1S/C11H20O3/c1-3-7-10(12)8-5-6-9-11(13)14-4-2/h3-9H2,1-2H3
InchiKey: NXLGAXQMRZRNRB-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CCCC(=O)CCCCC(=O)OCC
Mol. weight [g/mol]: 200.27
CAS: 4144-59-6

Physical Properties

Property code	Value	Unit	Source
gf	-321.10	kJ/mol	Joback Method
hf	-627.75	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	55.98	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.479		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
tb	581.24	K	Joback Method
tc	760.51	K	Joback Method
tf	335.82	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.66	J/mol×K	581.24	Joback Method
cpg	452.74	J/mol×K	611.12	Joback Method
cpg	466.22	J/mol×K	641.00	Joback Method
cpg	479.10	J/mol×K	670.88	Joback Method
cpg	491.38	J/mol×K	700.76	Joback Method
cpg	503.08	J/mol×K	730.63	Joback Method
cpg	514.20	J/mol×K	760.51	Joback Method
dvisc	0.0025267	Pa×s	335.82	Joback Method

dvisc	0.0013404	Pa×s	376.72	Joback Method
dvisc	0.0008051	Pa×s	417.63	Joback Method
dvisc	0.0005296	Pa×s	458.53	Joback Method
dvisc	0.0003732	Pa×s	499.43	Joback Method
dvisc	0.0002772	Pa×s	540.34	Joback Method
dvisc	0.0002147	Pa×s	581.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4144596&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume