Nonanoic acid, 9-oxo-, methyl ester

Other names:	Azelaaldehydic acid, methyl ester
	Methyl azelaaldehydate
	Methyl 8-formyloctanoate
	Methyl 9-oxononanoate
	9-Oxononanoic acid methyl ester
Inchi:	InChI=1S/C10H18O3/c1-13-10(12)8-6-4-2-3-5-7-9-11/h9H,2-8H2,1H3
InchiKey:	JMLYDLZRFNYHHO-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	COC(=O)CCCCCCCC=O
Mol. weight [g/mol]:	186.25
CAS:	1931-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-300.12	kJ/mol	Joback Method
hf	-580.11	kJ/mol	Joback Method
hfus	26.73	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.089		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
tb	553.15	K	Joback Method
tc	730.17	K	Joback Method
tf	316.62	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.85	J/mol×K	553.15	Joback Method

cpg	403.90	J/mol×K	582.65	Joback Method
cpg	416.40	J/mol×K	612.16	Joback Method
cpg	428.36	J/mol×K	641.66	Joback Method
cpg	439.81	J/mol×K	671.16	Joback Method
cpg	450.73	J/mol×K	700.67	Joback Method
cpg	461.13	J/mol×K	730.17	Joback Method
dvisc	0.0029976	Pa×s	316.62	Joback Method
dvisc	0.0015901	Pa×s	356.04	Joback Method
dvisc	0.0009572	Pa×s	395.46	Joback Method
dvisc	0.0006317	Pa×s	434.88	Joback Method
dvisc	0.0004467	Pa×s	474.31	Joback Method
dvisc	0.0003332	Pa×s	513.73	Joback Method
dvisc	0.0002591	Pa×s	553.15	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1931631&Units=SI

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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