9-Oxononanoic acid

Inchi:	InChI=1S/C9H16O3/c10-8-6-4-2-1-3-5-7-9(11)12/h8H,1-7H2,(H,11,12)
InchiKey:	WLGDDELKYAWBBL-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	O=CCCCCCCCC(=O)O
Mol. weight [g/mol]:	172.22
CAS:	2553-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-340.36	kJ/mol	Joback Method
hf	-579.48	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	65.77	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.001		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
tb	600.03	K	Joback Method
tc	772.51	K	Joback Method
tf	343.94	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.39	J/mol×K	600.03	Joback Method
cpg	383.98	J/mol×K	628.78	Joback Method
cpg	394.08	J/mol×K	657.52	Joback Method
cpg	403.72	J/mol×K	686.27	Joback Method
cpg	412.89	J/mol×K	715.02	Joback Method
cpg	421.63	J/mol×K	743.76	Joback Method
cpg	429.94	J/mol×K	772.51	Joback Method

dvisc	0.0072689	Pa×s	343.94	Joback Method
dvisc	0.0025072	Pa×s	386.62	Joback Method
dvisc	0.0010686	Pa×s	429.30	Joback Method
dvisc	0.0005314	Pa×s	471.99	Joback Method
dvisc	0.0002967	Pa×s	514.67	Joback Method
dvisc	0.0001812	Pa×s	557.35	Joback Method
dvisc	0.0001187	Pa×s	600.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2553175&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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