

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:	WLGDELKYAWBBL-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/molxK	600.03	Joback Method
cpg	383.98	J/molxK	628.78	Joback Method
cpg	394.08	J/molxK	657.52	Joback Method
cpg	403.72	J/molxK	686.27	Joback Method
cpg	412.89	J/molxK	715.02	Joback Method
cpg	421.63	J/molxK	743.76	Joback Method
cpg	429.94	J/molxK	772.51	Joback Method

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2553175&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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