Alpha-nonenoic acid

Other names:	Nonylenic acid
	2-Nonenylic acid
	«alpha»-Nonenoic acid
	Alpha-nonenoic acid
	trans-2-Nonenoic acid
	non-2-enoic acid
Inchi:	InChI=1S/C9H16O2/c1-2-3-4-5-6-7-8-9(10)11/h7-8H,2-6H2,1H3,(H,10,11)/b8-7+
InchiKey:	ADLXTJMPCFOTOO-BQYQJAHWSA-N
Formula:	C9H16O2
SMILES:	CCCCCC/C=C/C(=O)O
Mol. weight [g/mol]:	156.23

Physical Properties

Property code	Value	Unit	Source
af	0.7438		Cheméo Relay (1.0)
gf	-160.62	kJ/mol	Joback Method
hf	-483.32	kJ/mol	Cheméo Relay (1.0)
hfus	24.96	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Cheméo Relay (1.0)
ie	9.91	eV	Cheméo Relay (1.0)
log10ws	-3.29		Cheméo Relay (1.0)
logp	2.598		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1321.00		NIST Webbook
tb	526.91	K	Cheméo Relay (1.0)
tc	701.63	K	Cheméo Relay (1.0)
tf	327.08	K	Cheméo Relay (1.0)
vc	0.501	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.19	J/mol×K	555.53	Joback Method

cpg	347.39	J/mol×K	584.59	Joback Method
cpg	358.07	J/mol×K	613.65	Joback Method
cpg	368.24	J/mol×K	642.71	Joback Method
cpg	377.94	J/mol×K	671.77	Joback Method
cpg	387.18	J/mol×K	700.83	Joback Method
cpg	395.99	J/mol×K	729.89	Joback Method
dvisc	0.0133879	Pa×s	296.86	Joback Method
dvisc	0.0035614	Pa×s	339.97	Joback Method
dvisc	0.0012764	Pa×s	383.08	Joback Method
dvisc	0.0005630	Pa×s	426.19	Joback Method
dvisc	0.0002886	Pa×s	469.31	Joback Method
dvisc	0.0001656	Pa×s	512.42	Joback Method
dvisc	0.0001035	Pa×s	555.53	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3760110&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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