

non-1-en-4-one

Inchi:	InChI=1S/C9H16O/c1-3-5-6-8-9(10)7-4-2/h4H,2-3,5-8H2,1H3
InchiKey:	WDBHYTAEQAWRCQ-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	C=CCC(=O)CCCC
Mol. weight [g/mol]:	140.22

Physical Properties

Property code	Value	Unit	Source
gf	-16.18	kJ/mol	Joback Method
hf	-216.24	kJ/mol	Joback Method
hfus	19.38	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mvol	134.940	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1044.00		NIST Webbook
ripol	1347.00		NIST Webbook
tb	455.87	K	Joback Method
tc	633.46	K	Joback Method
tf	239.36	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.91	J/molxK	455.87	Joback Method
cpg	340.27	J/molxK	603.86	Joback Method
cpg	329.45	J/molxK	574.26	Joback Method
cpg	318.12	J/molxK	544.67	Joback Method
cpg	306.26	J/molxK	515.07	Joback Method
cpg	293.86	J/molxK	485.47	Joback Method
cpg	350.60	J/molxK	633.46	Joback Method
dvisc	0.0002840	Paxs	455.87	Joback Method

dvisc	0.0003655	Paxs	419.79	Joback Method
dvisc	0.0004934	Paxs	383.70	Joback Method
dvisc	0.0007087	Paxs	347.62	Joback Method
dvisc	0.0011072	Paxs	311.53	Joback Method
dvisc	0.0019443	Paxs	275.44	Joback Method
dvisc	0.0040460	Paxs	239.36	Joback Method

Sources

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=R217368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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