

(Z)-3-nonenal

Inchi: InChI=1S/C9H16O/c1-2-3-4-5-6-7-8-9-10/h6-7,9H,2-5,8H2,1H3/b7-6-
InchiKey: YXEAENVLZOODMT-SREVYHEPSA-N
Formula: C9H16O
SMILES: CCCCCC=CCC=O
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
gf	5.60	kJ/mol	Joback Method
hf	-197.45	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	458.14	K	Joback Method
tc	635.79	K	Joback Method
tf	228.11	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.56	J/mol×K	458.14	Joback Method
cpg	341.26	J/mol×K	606.18	Joback Method
cpg	330.61	J/mol×K	576.57	Joback Method
cpg	319.44	J/mol×K	546.97	Joback Method
cpg	307.72	J/mol×K	517.36	Joback Method
cpg	295.43	J/mol×K	487.75	Joback Method
cpg	351.41	J/mol×K	635.79	Joback Method
dvisc	0.0002551	Pa×s	458.14	Joback Method
dvisc	0.0003323	Pa×s	419.80	Joback Method
dvisc	0.0004566	Pa×s	381.46	Joback Method
dvisc	0.0006735	Pa×s	343.12	Joback Method
dvisc	0.0010953	Pa×s	304.79	Joback Method
dvisc	0.0020491	Pa×s	266.45	Joback Method
dvisc	0.0047317	Pa×s	228.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R298590&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

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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