

(Z,Z)-3,6-Nonadienal

Other names:	(3Z,6Z)-3,6-Nonadienal 3,6-Nonadienal, (Z,Z)- (Z,Z)-3,6-Nonadienal cis,cis-3,6-Nonadienal
Inchi:	InChI=1S/C9H14O/c1-2-3-4-5-6-7-8-9-10/h3-4,6-7,9H,2,5,8H2,1H3/b4-3-,7-6-
InchiKey:	FIDBXHOCOXRPRO-CWWKMNTPSA-N
Formula:	C9H14O
SMILES:	CCC=CCC=CCC=O
Mol. weight [g/mol]:	138.21
CAS:	21944-83-2

Physical Properties

Property code	Value	Unit	Source
gf	85.82	kJ/mol	Joback Method
hf	-80.23	kJ/mol	Joback Method
hfus	21.76	kJ/mol	Joback Method
hvap	42.26	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.488		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	462.30	K	Joback Method
tc	648.39	K	Joback Method
tf	223.03	K	Joback Method
vc	0.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.24	J/molxK	462.30	Joback Method
cpg	322.54	J/molxK	617.38	Joback Method
cpg	312.48	J/molxK	586.36	Joback Method
cpg	301.85	J/molxK	555.35	Joback Method
cpg	290.63	J/molxK	524.33	Joback Method
cpg	278.77	J/molxK	493.32	Joback Method
cpg	332.06	J/molxK	648.39	Joback Method
dvisc	0.0002135	Paxs	462.30	Joback Method
dvisc	0.0002786	Paxs	422.42	Joback Method
dvisc	0.0003843	Paxs	382.54	Joback Method
dvisc	0.0005712	Paxs	342.66	Joback Method
dvisc	0.0009426	Paxs	302.79	Joback Method
dvisc	0.0018105	Paxs	262.91	Joback Method
dvisc	0.0043918	Paxs	223.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21944832&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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