

(E,Z,Z)-2,4,6-nonatrienal

Inchi:	InChI=1S/C9H12O/c1-2-3-4-5-6-7-8-9-10/h3-9H,2H2,1H3/b4-3+,6-5-,8-7+
InchiKey:	XHDSWFFUGPJMMN-GFCVGDUSA-N
Formula:	C9H12O
SMILES:	CCC=CC=CC=CC=O
Mol. weight [g/mol]:	136.19

Physical Properties

Property code	Value	Unit	Source
gf	166.04	kJ/mol	Joback Method
hf	36.99	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hvap	42.22	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.264		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
ripol	1841.00		NIST Webbook
ripol	1841.00		NIST Webbook
ripol	1845.00		NIST Webbook
tb	466.46	K	Joback Method
tc	661.54	K	Joback Method
tf	217.95	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.68	J/molxK	466.46	Joback Method
cpg	261.80	J/molxK	498.97	Joback Method
cpg	273.16	J/molxK	531.49	Joback Method
cpg	283.82	J/molxK	564.00	Joback Method
cpg	293.82	J/molxK	596.51	Joback Method
cpg	303.21	J/molxK	629.02	Joback Method
cpg	312.04	J/molxK	661.54	Joback Method

dvisc	0.0040805	Paxs	217.95	Joback Method
dvisc	0.0015983	Paxs	259.37	Joback Method
dvisc	0.0008104	Paxs	300.79	Joback Method
dvisc	0.0004843	Paxs	342.20	Joback Method
dvisc	0.0003235	Paxs	383.62	Joback Method
dvisc	0.0002337	Paxs	425.04	Joback Method
dvisc	0.0001789	Paxs	466.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R315096&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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