(E,E,E)-2,4,6-Nonatrienal

Other names: all-(E)-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-ARQDATDDSA-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
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1896.00		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/mol×K	466.46	Joback Method
cpg	261.80	J/mol×K	498.97	Joback Method
cpg	273.16	J/mol×K	531.49	Joback Method
cpg	283.82	J/mol×K	564.00	Joback Method

cpg	293.82	J/mol×K	596.51	Joback Method
cpg	303.21	J/mol×K	629.02	Joback Method
cpg	312.04	J/mol×K	661.54	Joback Method
dvisc	0.0040805	Pa×s	217.95	Joback Method
dvisc	0.0015983	Pa×s	259.37	Joback Method
dvisc	0.0008104	Pa×s	300.79	Joback Method
dvisc	0.0004843	Pa×s	342.20	Joback Method
dvisc	0.0003235	Pa×s	383.62	Joback Method
dvisc	0.0002337	Pa×s	425.04	Joback Method
dvisc	0.0001789	Pa×s	466.46	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R417924&Units=SI

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