2(E),6(Z)-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-WWVFNRLHSA-N
Formula: C9H14O
SMILES: CCC=CCC=CCC=O
Mol. weight [g/mol]: 138.21

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	1155.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	462.30	K	Joback Method
tc	648.39	K	Joback Method
tf	223.03	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.24	J/mol×K	462.30	Joback Method
cpg	278.77	J/mol×K	493.32	Joback Method
cpg	290.63	J/mol×K	524.33	Joback Method
cpg	301.85	J/mol×K	555.35	Joback Method
cpg	312.48	J/mol×K	586.36	Joback Method

cpg	322.54	J/mol×K	617.38	Joback Method
cpg	332.06	J/mol×K	648.39	Joback Method
dvisc	0.0043918	Pa×s	223.03	Joback Method
dvisc	0.0018105	Pa×s	262.91	Joback Method
dvisc	0.0009426	Pa×s	302.79	Joback Method
dvisc	0.0005712	Pa×s	342.66	Joback Method
dvisc	0.0003843	Pa×s	382.54	Joback Method
dvisc	0.0002786	Pa×s	422.42	Joback Method
dvisc	0.0002135	Pa×s	462.30	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=R615044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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