2-Nonenal, dimethylacetal

Inchi: InChI=1S/C11H22O2/c1-4-5-6-7-8-9-10-11(12-2)13-3/h9-11H,4-8H2,1-3H3/b10-9+
InchiKey: VKWXFMOLPWWLDR-MDZDMXLPSA-N
Formula: C11H22O2
SMILES: CCCCCCC=CC(OC)OC
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-90.48	kJ/mol	Joback Method
hf	-422.87	kJ/mol	Joback Method
hfus	23.30	kJ/mol	Joback Method
hvap	44.47	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.132		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1666.00		NIST Webbook
tb	499.64	K	Joback Method
tc	671.60	K	Joback Method
tf	238.11	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.23	J/mol×K	499.64	Joback Method
cpg	414.75	J/mol×K	528.30	Joback Method
cpg	429.70	J/mol×K	556.96	Joback Method
cpg	444.09	J/mol×K	585.62	Joback Method
cpg	457.92	J/mol×K	614.28	Joback Method
cpg	471.19	J/mol×K	642.94	Joback Method

cpg	483.93	J/mol×K	671.60	Joback Method
dvisc	0.0042645	Pa×s	238.11	Joback Method
dvisc	0.0015033	Pa×s	281.70	Joback Method
dvisc	0.0007008	Pa×s	325.29	Joback Method
dvisc	0.0003913	Pa×s	368.88	Joback Method
dvisc	0.0002471	Pa×s	412.46	Joback Method
dvisc	0.0001704	Pa×s	456.05	Joback Method
dvisc	0.0001253	Pa×s	499.64	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R409255&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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