6-Nonenal, 3,7-dimethyl-

Inchi: InChI=1S/C11H20O/c1-4-10(2)6-5-7-11(3)8-9-12/h6,9,11H,4-5,7-8H2,1-3H3/b10-6+
InchiKey: JFFUZMNCDKUJSH-UXBLZVDNSA-N
Formula: C11H20O
SMILES: CCC(C)=CCCC(C)CC=O
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
gf	11.45	kJ/mol	Joback Method
hf	-253.80	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	46.45	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.348		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
tb	503.34	K	Joback Method
tc	684.65	K	Joback Method
tf	221.69	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.60	J/mol×K	503.34	Joback Method
cpg	386.77	J/mol×K	533.56	Joback Method
cpg	401.23	J/mol×K	563.78	Joback Method
cpg	415.01	J/mol×K	593.99	Joback Method
cpg	428.12	J/mol×K	624.21	Joback Method
cpg	440.61	J/mol×K	654.43	Joback Method
cpg	452.49	J/mol×K	684.65	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=U132439&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume