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
InchiKey: JFFUZMNCDKUJSH-UXBLZVDNSA-N
Formula: C11H20O
SMILES: CC/C(C)=C/CCC(C)CC=O
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
hfus	21.90	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
logp	3.348		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
tb	488.27	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U132439&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature