(E)-2-Methyl-2-nonenal

Inchi: InChI=1S/C10H18O/c1-3-4-5-6-7-8-10(2)9-11/h8-9H,3-7H2,1-2H3/b10-8+
InchiKey: LLKFVNRSHSPYML-CSKARUKUSA-N
Formula: C10H18O
SMILES: CCCCCCC=C(C)C=O
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	5.47	kJ/mol	Joback Method
hf	-227.88	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.102		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1218.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
tb	480.90	K	Joback Method
tc	660.20	K	Joback Method
tf	225.42	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.96	J/mol×K	480.90	Joback Method
cpg	339.96	J/mol×K	510.78	Joback Method
cpg	353.30	J/mol×K	540.67	Joback Method
cpg	366.02	J/mol×K	570.55	Joback Method
cpg	378.15	J/mol×K	600.43	Joback Method
cpg	389.70	J/mol×K	630.31	Joback Method

cpg	400.71	J/mol×K	660.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434632&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

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
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

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