2,4-Dimethyl-2,4-hexadienal, not E,E, # 1

Inchi: InChI=1S/C8H12O/c1-4-7(2)5-8(3)6-9/h4-6H,1-3H3
InchiKey: JLRXGFYYIORWGF-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC=C(C)C=C(C)C=O
Mol. weight [g/mol]: 124.18

Physical Properties

Property code	Value	Unit	Source
gf	60.30	kJ/mol	Joback Method
hf	-79.17	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
tb	439.18	K	Joback Method
tc	634.54	K	Joback Method
tf	183.84	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.08	J/mol×K	439.18	Joback Method
cpg	236.97	J/mol×K	471.74	Joback Method
cpg	248.18	J/mol×K	504.30	Joback Method
cpg	258.74	J/mol×K	536.86	Joback Method
cpg	268.70	J/mol×K	569.42	Joback Method
cpg	278.09	J/mol×K	601.98	Joback Method
cpg	286.95	J/mol×K	634.54	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=R597614&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
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