(Z)-3,7-dimethyl-3,6-octadienal

Inchi: InChI=1S/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5-6,8H,4,7H2,1-3H3/b10-6-
InchiKey: OJLMARCQPSGYNE-POHAHGRESA-N
Formula: C10H16O
SMILES: CC(C)=CCC=C(C)CC=O
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	77.14	kJ/mol	Joback Method
hf	-120.45	kJ/mol	Joback Method
hfus	21.73	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.878		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1151.00		NIST Webbook
rinpol	1165.30		NIST Webbook
rinpol	1175.00		NIST Webbook
tb	484.94	K	Joback Method
tc	675.98	K	Joback Method
tf	206.38	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.04	J/mol×K	484.94	Joback Method
cpg	322.90	J/mol×K	516.78	Joback Method
cpg	336.01	J/mol×K	548.62	Joback Method
cpg	348.41	J/mol×K	580.46	Joback Method
cpg	360.14	J/mol×K	612.30	Joback Method
cpg	371.25	J/mol×K	644.14	Joback Method
cpg	381.76	J/mol×K	675.98	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=U414180&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume