(2E,4E)-6-Hydroxy-2,6-dimethylhepta-2,4-dienal

Inchi: InChI=1S/C9H14O2/c1-8(7-10)5-4-6-9(2,3)11/h4-7,11H,1-3H3/b6-4+,8-5+
InchiKey: VMRUOMPSDZHKQS-HLQBBKRNSA-N
Formula: C9H14O2
SMILES: CC(C=O)=CC=CC(C)(C)O
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-56.71	kJ/mol	Joback Method
hf	-251.00	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	57.73	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.459		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1275.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2173.00		NIST Webbook
tb	551.13	K	Joback Method
tc	741.45	K	Joback Method
tf	272.31	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.39	J/mol×K	551.13	Joback Method
cpg	332.60	J/mol×K	582.85	Joback Method
cpg	343.09	J/mol×K	614.57	Joback Method
cpg	352.92	J/mol×K	646.29	Joback Method
cpg	362.14	J/mol×K	678.01	Joback Method
cpg	370.80	J/mol×K	709.73	Joback Method
cpg	378.96	J/mol×K	741.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228794&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