3,4-Pentadienal, 2,2-dimethyl-

Other names: 2,2-Dimethyl 3,4-pentadienal
Inchi: InChI=1S/C7H10O/c1-4-5-7(2,3)6-8/h5-6H,1H2,2-3H3
InchiKey: QAMJLJHOJKMLEU-UHFFFAOYSA-N
Formula: C7H10O
SMILES: C=C=CC(C)(C)C=O
Mol. weight [g/mol]: 110.15
CAS: 4058-51-9

Physical Properties

Property code	Value	Unit	Source
gf	127.50	kJ/mol	Joback Method
hf	6.07	kJ/mol	Joback Method
hfus	9.61	kJ/mol	Joback Method
hvap	36.37	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.553		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
ripol	1573.00		NIST Webbook
tb	404.94	K	Joback Method
tc	604.21	K	Joback Method
tf	217.82	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.72	J/mol×K	404.94	Joback Method
cpg	204.42	J/mol×K	438.15	Joback Method
cpg	214.54	J/mol×K	471.36	Joback Method
cpg	224.10	J/mol×K	504.58	Joback Method
cpg	233.13	J/mol×K	537.79	Joback Method
cpg	241.65	J/mol×K	571.00	Joback Method
cpg	249.67	J/mol×K	604.21	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=C4058519&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume