2-Isopropylidene-3-methylhexa-3,5-dienal

Inchi: InChI=1S/C10H14O/c1-5-6-9(4)10(7-11)8(2)3/h5-7H,1H2,2-4H3/b9-6+
InchiKey: NIEPGDUXTWPJLS-RMKNXTFCSA-N
Formula: C10H14O
SMILES: C=CC=C(C)C(C=O)=C(C)C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	156.43	kJ/mol	Joback Method
hf	-4.81	kJ/mol	Joback Method
hfus	19.14	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
tb	481.50	K	Joback Method
tc	680.24	K	Joback Method
tf	190.66	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.44	J/mol×K	481.50	Joback Method
cpg	304.90	J/mol×K	514.62	Joback Method
cpg	317.56	J/mol×K	547.75	Joback Method
cpg	329.47	J/mol×K	580.87	Joback Method
cpg	340.67	J/mol×K	613.99	Joback Method
cpg	351.22	J/mol×K	647.12	Joback Method
cpg	361.15	J/mol×K	680.24	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=U191765&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