2-Hexenal, 4-methyl-2-phenyl

Inchi: InChI=1S/C14H18O/c1-3-7-12(2)10-14(11-15)13-8-5-4-6-9-13/h4-6,8-12H,3,7H2,1-2H3/b
InchiKey: JDIPTMQQKZUVBB-UVTDQMKNSA-N
Formula: C14H18O
SMILES: CCCC(C)C=C(C=O)c1ccccc1
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	149.12	kJ/mol	Joback Method
hf	-79.19	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	55.40	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.705		Crippen Method
mcvol	181.630	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1433.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1433.00		NIST Webbook
tb	598.66	K	Joback Method
tc	812.17	K	Joback Method
tf	281.92	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.27	J/mol×K	598.66	Joback Method
cpg	463.83	J/mol×K	634.24	Joback Method
cpg	479.32	J/mol×K	669.83	Joback Method
cpg	493.81	J/mol×K	705.41	Joback Method
cpg	507.36	J/mol×K	741.00	Joback Method
cpg	520.05	J/mol×K	776.58	Joback Method

cpg	531.91	J/mol×K	812.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R45756&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume