2-Hexenal, 5-methyl-2-phenyl

Inchi: InChI=1S/C14H18O/c1-3-12(2)9-10-14(11-15)13-7-5-4-6-8-13/h4-8,10-12H,3,9H2,1-2H3
InchiKey: BOJMHRVYPALVNQ-UVTDQMKNSA-N
Formula: C14H18O
SMILES: CCC(C)CC=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	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1495.00		NIST Webbook
ripol	2000.00		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=R45710&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