Octanal, 2-(phenylmethylene)-

Other names:	Cinnamaldehyde, «alpha»-hexyl-
	«alpha»-n-Hexyl-«beta»-phenylacrolein
	«alpha»-Hexylcinnamaldehyde
	«alpha»-Hexylcinnamic aldehyde
	Hexyl cinnamic aldehyde
	2-Hexyl-3-phenyl-2-propenal
	2-Hexyl-3-phenyl-propenal
	n-Hexyl cinnamaldehyde
	2-(Phenylmethylene)octanal
	2-Hexylcinnamaldehyde
	NSC 406799
	«alpha»-Hexylcinnamyl aldehyde
	Hexylcinnamaldehyde
Inchi:	InChI=1S/C15H20O/c1-2-3-4-6-11-15(13-16)12-14-9-7-5-8-10-14/h5,7-10,12-13H,2-4,6,1
InchiKey:	GUUHFMWKWLOQMM-QINSGFPZSA-N
Formula:	C15H20O
SMILES:	CCCCCCC(C=O)=Cc1ccccc1
Mol. weight [g/mol]:	216.32
CAS:	101-86-0

Physical Properties

Property code	Value	Unit	Source
gf	159.98	kJ/mol	Joback Method
hf	-94.55	kJ/mol	Joback Method
hfus	29.83	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.239		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1764.00		NIST Webbook

rinpol	1765.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1726.20		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1726.20		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1766.00		NIST Webbook
ripol	2309.00		NIST Webbook
tb	621.98	K	Joback Method
tc	827.96	K	Joback Method
tf	308.19	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.60	J/mol×K	621.98	Joback Method
cpg	514.24	J/mol×K	656.31	Joback Method
cpg	529.87	J/mol×K	690.64	Joback Method
cpg	544.54	J/mol×K	724.97	Joback Method
cpg	558.31	J/mol×K	759.30	Joback Method
cpg	571.25	J/mol×K	793.63	Joback Method
cpg	583.40	J/mol×K	827.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.20	K	2.00	NIST Webbook

Sources

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=C101860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume