Cinnamaldehyde, «alpha»-pentyl-

Other names:	Heptanal, 2-(phenylmethylene)-
	«alpha»-Amyl-«beta»-phenylacrolein
	«alpha»-Amylcinnamaldehyde
	«alpha»-Pentylcinnamaldehyde
	Amylcinnamaldehyde
	Flomine
	Jasminal
	Jasminaldehyde
	«alpha»-Amylcinnamic aldehyde
	«alpha»-n-Amylcinnamaldehyde
	Amylcinnamic aldehyde
	Heptanal, 2-benzylidene-
	«alpha»-n-Amylcinnamic aldehyde
	2-(Phenylmethylene)heptanal
	2-Benzylideneheptanal
	Amylcinnamic acid aldehyde
	Cinnamaldehyde, «alpha»-amyl-
	Jasmine aldehyde
	NSC 6649
	Pentylcinnamaldehyde
	Amyl cinnamal
	Jasmal
Inchi:	InChI=1S/C14H18O/c1-2-3-5-10-14(12-15)11-13-8-6-4-7-9-13/h4,6-9,11-12H,2-3,5,10H2
InchiKey:	HMKKIXGYKWDQSV-KAMYIIQDSA-N
Formula:	C14H18O
SMILES:	CCCCCC(C=O)=Cc1ccccc1
Mol. weight [g/mol]:	202.29
CAS:	122-40-7

Physical Properties

Property code	Value	Unit	Source
gf	151.56	kJ/mol	Joback Method
hf	-73.91	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method

logp	3.849		Crippen Method
mcvol	181.630	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1615.10		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1615.10		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2247.00		NIST Webbook
tb	561.70	K	NIST Webbook
tc	808.30	K	Joback Method
tf	296.92	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.88	J/mol×K	599.10	Joback Method
cpg	463.04	J/mol×K	633.97	Joback Method
cpg	478.20	J/mol×K	668.83	Joback Method
cpg	492.41	J/mol×K	703.70	Joback Method
cpg	505.72	J/mol×K	738.57	Joback Method
cpg	518.21	J/mol×K	773.44	Joback Method
cpg	529.91	J/mol×K	808.30	Joback Method
hvapt	75.30	kJ/mol	307.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.70	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122407&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
hvapt:	Enthalpy of vaporization at a given temperature
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