2-Propenal, 2-methyl-3-phenyl-

Other names:	Cinnamaldehyde, «alpha»-methyl-
	«alpha»-Methylcinnamaldehyde
	«alpha»-Methylcinnamic aldehyde
	2-Methyl-3-phenylacrolein
	2-Methyl-3-phenylacrylaldehyde
	«alpha»-Methylcinnimal
	Methyl cinnamic aldehyde
	2-Methyl-3-phenyl-2-propenal
	Cinnamic aldehyde, «alpha»-methyl
	2-Methyl-3-phenylpropenal
	2-Methylcinnamaldehyde
	NSC 22283
Inchi:	InChI=1S/C10H10O/c1-9(8-11)7-10-5-3-2-4-6-10/h2-8H,1H3/b9-7+
InchiKey:	VLUMOWNVWOXZAU-VQHVLOKHSA-N
Formula:	C10H10O
SMILES:	CC(C=O)=Cc1ccccc1
Mol. weight [g/mol]:	146.19
CAS:	101-39-3

Physical Properties

Property code	Value	Unit	Source
gf	117.88	kJ/mol	Joback Method
hf	8.65	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	46.89	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.289		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1330.00		NIST Webbook
ripol	1992.00		NIST Webbook
ripol	1992.00		NIST Webbook
ripol	1992.00		NIST Webbook
tb	507.58	K	Joback Method

tc	731.50	K	Joback Method
tf	251.84	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.82	J/mol×K	507.58	Joback Method
cpg	317.40	J/mol×K	694.18	Joback Method
cpg	307.53	J/mol×K	656.86	Joback Method
cpg	296.89	J/mol×K	619.54	Joback Method
cpg	285.43	J/mol×K	582.22	Joback Method
cpg	273.09	J/mol×K	544.90	Joback Method
cpg	326.56	J/mol×K	731.50	Joback Method
hvapt	71.50	kJ/mol	368.00	NIST Webbook
hvapt	47.70 ± 0.60	kJ/mol	478.50	NIST Webbook
hvapt	50.50 ± 0.40	kJ/mol	478.50	NIST Webbook
hvapt	53.40 ± 0.20	kJ/mol	478.50	NIST Webbook
hvapt	56.30 ± 0.20	kJ/mol	478.50	NIST Webbook
hvapt	59.30 ± 0.20	kJ/mol	478.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.70	K	3.60	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=C101393&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
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