Phenylpropynal

Other names:	Phenylpropargyl aldehyde
	2-Propynal, 3-phenyl-
	Benzenepropiolaldehyde
	Phenylacetylenecarboxaldehyde
	Phenylpropiolaldehyde
	Propiolaldehyde, phenyl-
	3-Phenyl-2-propynal
	3-Phenylpropynal
	NSC 47568
Inchi:	InChI=1S/C9H6O/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,8H
InchiKey:	IDASOVSVRKONFS-UHFFFAOYSA-N
Formula:	C9H6O
SMILES:	O=CC#Cc1ccccc1
Mol. weight [g/mol]:	130.14
CAS:	2579-22-8

Physical Properties

Property code	Value	Unit	Source
chl	-4527.90	kJ/mol	NIST Webbook
gf	240.59	kJ/mol	Joback Method
hf	194.16	kJ/mol	Joback Method
hfl	128.80 ± 4.00	kJ/mol	NIST Webbook
hfl	-104.00	kJ/mol	NIST Webbook
hfus	18.52	kJ/mol	Joback Method
hvap	46.78	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.237		Crippen Method
mcvol	106.880	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	489.66	K	Joback Method
tc	732.64	K	Joback Method
tf	365.71	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.95	J/mol×K	489.66	Joback Method
cpg	213.11	J/mol×K	530.16	Joback Method
cpg	223.48	J/mol×K	570.65	Joback Method
cpg	233.09	J/mol×K	611.15	Joback Method
cpg	241.99	J/mol×K	651.65	Joback Method
cpg	250.22	J/mol×K	692.14	Joback Method
cpg	257.81	J/mol×K	732.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.20	K	1.70	NIST Webbook
tbrp	400.70	K	3.70	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2579228&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume