PHENYLPROPIOLIC ACID

Other names:	Phenylacetylenecarboxylic acid
	3-Phenylpropynoic acid
	2-Propynoic acid, 3-phenyl-
	Phenylacetylene monocarboxylic acid
	Phenylpropynoic acid
	Propiolic acid, phenyl-
	Propiolic acid, 3-phenyl-
	3-Phenylpropiolic acid
	«beta»-Phenylpropargylic acid
	3-Phenylpropargylic acid
	NSC 13669
Inchi:	InChI=1S/C9H6O2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,(H,10,11)
InchiKey:	XNERWVPQCYSMLC-UHFFFAOYSA-N
Formula:	C9H6O2
SMILES:	O=C(O)C#Cc1ccccc1
Mol. weight [g/mol]:	146.15

Physical Properties

Property code	Value	Unit	Source
chs	-4277.30	kJ/mol	NIST Webbook
hf	-75.78	kJ/mol	Cheméo Relay (1.0)
hfl	-121.80 ± 4.00	kJ/mol	NIST Webbook
hfs	146.00	kJ/mol	NIST Webbook
hfus	21.92	kJ/mol	Joback Method
hvap	78.26	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
logp	1.123		Crippen Method
mcvol	112.750	ml/mol	McGowan Method
tb	536.35	K	Cheméo Relay (1.0)
tf	410.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	241.34	J/mol×K	587.05	Joback Method
cpg	250.57	J/mol×K	625.10	Joback Method
cpg	259.14	J/mol×K	663.14	Joback Method
cpg	267.10	J/mol×K	701.19	Joback Method
cpg	274.46	J/mol×K	739.23	Joback Method
cpg	281.26	J/mol×K	777.28	Joback Method
cpg	287.54	J/mol×K	815.32	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C637445&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point