

Phenylpropionic 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-Phenylpropionic 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: XNERWVPQCYSMCLC-UHFFFAOYSA-N
Formula: C9H6O2
SMILES: O=C(O)C#Cc1ccccc1
Mol. weight [g/mol]: 146.14
CAS: 637-44-5

Physical Properties

Property code	Value	Unit	Source
chs	-4277.30	kJ/mol	NIST Webbook
gf	74.37	kJ/mol	Joback Method
hf	14.93	kJ/mol	Joback Method
hfl	-121.80 ± 4.00	kJ/mol	NIST Webbook
hfs	146.00	kJ/mol	NIST Webbook
hfus	21.92	kJ/mol	Joback Method
hvap	63.48	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.123		Crippen Method
mcvol	112.750	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	587.05	K	Joback Method
tc	815.32	K	Joback Method
tf	410.00 ± 2.00	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

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

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=C637445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid 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
hfs:	Solid 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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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