Benzenemethanol, «alpha»-ethynyl-

Other names:	Benzyl alcohol, «alpha»-ethynyl-
	«alpha»-Ethynylbenzyl alcohol
	«alpha»-Phenylpropargyl alcohol
	Phenylethynylcarbinol
	1-Phenylpropargyl alcohol
	2-Propyn-1-ol, 1-phenyl-
	1-Phenyl-2-propyn-1-ol
	1-Phenyl-2-propyne-1-ol
	Ethynylphenylcarbinol
	NSC 4326
	1-phenylprop-2-yn-1-ol
Inchi:	InChI=1S/C9H8O/c1-2-9(10)8-6-4-3-5-7-8/h1,3-7,9-10H
InchiKey:	UIGLAZDLBZDVBL-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	C#CC(O)c1ccccc1
Mol. weight [g/mol]:	132.16
CAS:	4187-87-5

Physical Properties

Property code	Value	Unit	Source
gf	221.12	kJ/mol	Joback Method
hf	141.83	kJ/mol	Joback Method
hfus	16.65	kJ/mol	Joback Method
hvap	54.05	kJ/mol	Joback Method
ie	10.69	eV	NIST Webbook
log10ws	-2.21		Crippen Method
logp	1.353		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	513.86	K	Joback Method
tc	727.25	K	Joback Method
tf	310.40	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.40	J/mol×K	513.86	Joback Method
cpg	242.80	J/mol×K	549.42	Joback Method
cpg	252.49	J/mol×K	584.99	Joback Method
cpg	261.52	J/mol×K	620.55	Joback Method
cpg	269.91	J/mol×K	656.12	Joback Method
cpg	277.71	J/mol×K	691.68	Joback Method
cpg	284.97	J/mol×K	727.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.00 ± 1.00	K	1.90	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=C4187875&Units=SI

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
ie:	Ionization energy
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

Latest version available from:

https://www.chemeo.com/cid/40-130-2/Benzenemethanol-alpha-ethynyl.pdf

Generated by Cheméo on 2024-10-12 03:49:15.068632674 +0000 UTC m=+3285817.705601925.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.