2-Phenyl-3-butyn-2-ol

Other names:	3-Hydroxy-3-phenyl-1-butyne Benzenemethanol, «alpha»-ethynyl-«alpha»-methyl- «alpha»-Ethynyl-«alpha»-methylbenzenemethanol Benzyl alcohol, «alpha»-ethynyl-«alpha»-methyl- Methylphenylethynylcarbinol 3-Butyn-2-ol, 2-phenyl- «alpha»-Ethynyl-«alpha»-methylbenzyl alcohol 3-Phenyl-butin-1-ol-(3) NSC 4329 2-Phenyl-2-hydroxy-3-butyne 2-phenylbut-3-yn-2-ol
Inchi:	InChI=1S/C10H10O/c1-3-10(2,11)9-7-5-4-6-8-9/h1,4-8,11H,2H3
InchiKey:	KSLSOBUAIFEGLT-UHFFFAOYSA-N
Formula:	C10H10O
SMILES:	C#CC(C)(O)c1ccccc1
Mol. weight [g/mol]:	146.19
CAS:	127-66-2

Physical Properties

Property code	Value	Unit	Source
gf	234.82	kJ/mol	Joback Method
hf	117.72	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	55.37	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.527		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	533.95	K	Joback Method
tc	752.59	K	Joback Method
tf	326.00 ± 3.00	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.68	J/mol×K	533.95	Joback Method
cpg	290.58	J/mol×K	570.39	Joback Method
cpg	301.55	J/mol×K	606.83	Joback Method
cpg	311.66	J/mol×K	643.27	Joback Method
cpg	320.98	J/mol×K	679.71	Joback Method
cpg	329.57	J/mol×K	716.15	Joback Method
cpg	337.50	J/mol×K	752.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.00	K	1.30	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=C127662&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
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