

Benzenemethanol, «alpha»-ethynyl-«alpha»-phenyl-

Other names:	Diphenylethynylcarbinol 1,1-Diphenylpropargyl alcohol 2-Propyn-1-ol, 1,1-diphenyl- 3,3-Diphenyl-3-hydroxy-1-propyne 1,1-Diphenyl-2-propyn-1-ol
Inchi:	InChI=1S/C15H12O/c1-2-15(16,13-9-5-3-6-10-13)14-11-7-4-8-12-14/h1,3-12,16H
InchiKey:	SMCLTAARQYTXLW-UHFFFAOYSA-N
Formula:	C15H12O
SMILES:	C#CC(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	208.26
CAS:	3923-52-2

Physical Properties

Property code	Value	Unit	Source
gf	389.33	kJ/mol	Joback Method
hf	251.05	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	68.78	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.556		Crippen Method
mcvol	171.960	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	675.03	K	Joback Method
tc	918.68	K	Joback Method
tf	421.86	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.73	J/molxK	675.03	Joback Method
cpg	450.33	J/molxK	715.64	Joback Method
cpg	462.71	J/molxK	756.25	Joback Method
cpg	474.00	J/molxK	796.86	Joback Method

cpg	484.32	J/mol×K	837.46	Joback Method
cpg	493.82	J/mol×K	878.07	Joback Method
cpg	502.61	J/mol×K	918.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.00	K	2.40	NIST Webbook
tbrp	414.00 ± 2.00	K	0.30	NIST Webbook

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=C3923522&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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