Benzenemethanol, «alpha»-phenyl-«alpha»-(2-phenylethynyl)-

Other names: 1,1,3-triphenylpropargyl alcohol
Diphenyl(phenylethynyl)carbinol

Inchi: InChI=1S/C21H16O/c22-21(19-12-6-2-7-13-19,20-14-8-3-9-15-20)17-16-18-10-4-1-5-11-

InchiKey: VWRQCJRTHKUVNF-UHFFFAOYSA-N

Formula: C21H16O

SMILES: OC(C#Cc1ccccc1)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 284.35

CAS: 1522-13-0

Physical Properties

Property code	Value	Unit	Source
chs	-10720.00	kJ/mol	NIST Webbook
gf	531.99	kJ/mol	Joback Method
hf	344.14	kJ/mol	Joback Method
hfs	194.30	kJ/mol	NIST Webbook
hfus	32.06	kJ/mol	Joback Method
hvap	86.70	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.974		Crippen Method
mcvol	232.740	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	857.87	K	Joback Method
tc	1124.23	K	Joback Method
tf	575.03	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.89	J/mol×K	857.87	Joback Method
cpg	679.03	J/mol×K	902.26	Joback Method
cpg	691.95	J/mol×K	946.66	Joback Method
cpg	703.88	J/mol×K	991.05	Joback Method
cpg	715.00	J/mol×K	1035.44	Joback Method

cpg	725.51	J/mol×K	1079.83	Joback Method
cpg	735.60	J/mol×K	1124.23	Joback Method

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=C1522130&Units=SI

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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume