Benzenemethanol, «alpha»,«alpha»-diphenyl-

Other names:	NSC 4050
	Triphenylmethyl alcohol
	Tritanol
	methanol, triphenyl-
	triphenylcarbinol
	triphenylmethanol
	trityl alcohol
Inchi:	InChI=1S/C19H16O/c20-19(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-
InchiKey:	LZTRCELOJRDYMQ-UHFFFAOYSA-N
Formula:	C19H16O
SMILES:	OC(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	260.33
CAS:	76-84-6

Physical Properties

Property code	Value	Unit	Source
chs	-9798.90	kJ/mol	NIST Webbook
chs	-9760.90 ± 2.20	kJ/mol	NIST Webbook
gf	312.35	kJ/mol	Joback Method
hf	113.12	kJ/mol	Joback Method
hfs	-2.50 ± 2.30	kJ/mol	NIST Webbook
hfs	35.50	kJ/mol	NIST Webbook
hfus	23.76	kJ/mol	Joback Method
hsub	121.80 ± 1.70	kJ/mol	NIST Webbook
hvap	80.10	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.971		Crippen Method
mcvol	213.160	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	633.20	K	NIST Webbook
tc	1055.05	K	Joback Method
tf	435.35 ± 0.30	K	NIST Webbook
tf	435.20	K	Energetics and structural properties of neutral and deprotonated phenyl carbinols
tf	433.65 ± 1.50	K	NIST Webbook
tf	399.00 ± 1.50	K	NIST Webbook

tf	435.60 ± 0.30	K	NIST Webbook
tf	434.65 ± 1.50	K	NIST Webbook
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.80	J/mol×K	803.11	Joback Method
cpg	621.09	J/mol×K	845.10	Joback Method
cpg	634.11	J/mol×K	887.09	Joback Method
cpg	646.03	J/mol×K	929.08	Joback Method
cpg	657.01	J/mol×K	971.07	Joback Method
cpg	667.22	J/mol×K	1013.06	Joback Method
cpg	676.83	J/mol×K	1055.05	Joback Method
cps	318.80	J/mol×K	298.50	NIST Webbook
dvisc	0.0010436	Pa×s	446.39	Joback Method
dvisc	0.0003490	Pa×s	505.84	Joback Method
dvisc	0.0001470	Pa×s	565.30	Joback Method
dvisc	0.0000730	Pa×s	624.75	Joback Method
dvisc	0.0000409	Pa×s	684.20	Joback Method
dvisc	0.0000252	Pa×s	743.66	Joback Method
dvisc	0.0000166	Pa×s	803.11	Joback Method
hfust	27.24	kJ/mol	441.10	NIST Webbook
hsubt	122.00	kJ/mol	363.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Energetics and structural properties of neutral and deprotonated phenyl carbinols: https://www.doi.org/10.1016/j.jct.2016.02.010

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=C76846&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
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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