p-Benzylphenol

Other names:	Phenol, 4-(phenylmethyl)-
	p-Cresol, «alpha»-phenyl-
	«alpha»-Phenyl-p-cresol
	p-Hydroxydiphenyl methane
	Fesiasept
	4-(Phenylmethyl)phenol
	4-Benzylphenol
	4-Hydroxydiphenylmethane
	4-Hydroxyditane
	AI3-1932
	NSC 8078
	7563-63-5
Inchi:	InChI=1S/C13H12O/c14-13-8-6-12(7-9-13)10-11-4-2-1-3-5-11/h1-9,14H,10H2
InchiKey:	HJSPWKGEPDZNLK-UHFFFAOYSA-N
Formula:	C13H12O
SMILES:	Oc1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]:	184.23
CAS:	101-53-1

Physical Properties

Property code	Value	Unit	Source
chs	-6774.00	kJ/mol	NIST Webbook
gf	128.78	kJ/mol	Joback Method
hf	63.51	kJ/mol	NIST Webbook
hfs	-54.00	kJ/mol	NIST Webbook
hfus	23.29	kJ/mol	Joback Method
hsub	117.50	kJ/mol	NIST Webbook
hsub	117.90	kJ/mol	NIST Webbook
hvap	62.10	kJ/mol	Joback Method
ie	8.45 ± 0.05	eV	NIST Webbook
log10ws	-3.12		Crippen Method
logp	2.983		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
rinpol	295.40		NIST Webbook
rinpol	295.40		NIST Webbook
tb	594.00 ± 1.00	K	NIST Webbook

tb	595.20	K	NIST Webbook
tc	885.31	K	Joback Method
tf	359.00	K	NIST Webbook
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.08	J/mol×K	885.31	Joback Method
cpg	377.22	J/mol×K	630.82	Joback Method
cpg	391.93	J/mol×K	673.23	Joback Method
cpg	405.41	J/mol×K	715.65	Joback Method
cpg	417.82	J/mol×K	758.06	Joback Method
cpg	429.29	J/mol×K	800.48	Joback Method
cpg	440.00	J/mol×K	842.89	Joback Method
dvisc	0.0000260	Pa×s	630.82	Joback Method
dvisc	0.0010953	Pa×s	400.83	Joback Method
dvisc	0.0004472	Pa×s	439.16	Joback Method
dvisc	0.0002108	Pa×s	477.49	Joback Method
dvisc	0.0001111	Pa×s	515.82	Joback Method
dvisc	0.0000640	Pa×s	554.16	Joback Method
dvisc	0.0000396	Pa×s	592.49	Joback Method
hsubt	97.40	kJ/mol	324.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	472.20	K	1.30	NIST Webbook
tbrp	428.50 ± 1.50	K	0.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101531&Units=SI

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume