Benzyl 4-hydroxybenzoate

Other names:	Benzyl p-hydroxybenzoate
	p-Hydroxybenzoic acid benzyl ester
	Benzoic acid, 4-hydroxy-, phenylmethyl ester
	Benzoic acid, p-hydroxy-, benzyl ester
	Benzyl paraben
	Benzyl Parasept
	Benzyl Tegosept
	Nipabenzyl
	Parosept
	Solbrol Z
	NSC 8080
	4-Hydroxybenzoic acid benzyl ester
Inchi:	InChI=1S/C14H12O3/c15-13-8-6-12(7-9-13)14(16)17-10-11-4-2-1-3-5-11/h1-9,15H,10H2
InchiKey:	MOZDKDIOPSPTBH-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	O=C(OCc1ccccc1)c1ccc(O)cc1
Mol. weight [g/mol]:	228.24
CAS:	94-18-8

Physical Properties

Property code	Value	Unit	Source
gf	-96.72	kJ/mol	Joback Method
hf	-281.34	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.749		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	729.99	K	Joback Method
tc	979.95	K	Joback Method
tf	484.26	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.36	J/mol×K	729.99	Joback Method
cpg	477.44	J/mol×K	771.65	Joback Method
cpg	489.51	J/mol×K	813.31	Joback Method
cpg	500.71	J/mol×K	854.97	Joback Method
cpg	511.14	J/mol×K	896.63	Joback Method
cpg	520.92	J/mol×K	938.29	Joback Method
cpg	530.18	J/mol×K	979.95	Joback Method
dvisc	0.0002882	Pa×s	484.26	Joback Method
dvisc	0.0001379	Pa×s	525.22	Joback Method
dvisc	0.0000734	Pa×s	566.17	Joback Method
dvisc	0.0000426	Pa×s	607.12	Joback Method
dvisc	0.0000264	Pa×s	648.08	Joback Method
dvisc	0.0000174	Pa×s	689.04	Joback Method
dvisc	0.0000120	Pa×s	729.99	Joback Method

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=C94188&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume