Benzyl 2-hydroxy-6-methoxybenzoate

Inchi: InChI=1S/C15H14O4/c1-18-13-9-5-8-12(16)14(13)15(17)19-10-11-6-3-2-4-7-11/h2-9,16H
InchiKey: CGNJMCLXIMWKDY-UHFFFAOYSA-N
Formula: C15H14O4
SMILES: COc1cccc(O)c1C(=O)OCc1ccccc1
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-202.93	kJ/mol	Joback Method
hf	-445.67	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	78.78	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.758		Crippen Method
mcvol	193.870	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	2046.00		NIST Webbook
tb	780.27	K	Joback Method
tc	1022.10	K	Joback Method
tf	530.28	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.38	J/mol×K	780.27	Joback Method
cpg	553.49	J/mol×K	820.57	Joback Method
cpg	565.67	J/mol×K	860.88	Joback Method
cpg	576.97	J/mol×K	901.18	Joback Method
cpg	587.49	J/mol×K	941.49	Joback Method
cpg	597.31	J/mol×K	981.79	Joback Method
cpg	606.51	J/mol×K	1022.10	Joback Method
dvisc	0.0001200	Pa×s	530.28	Joback Method
dvisc	0.0000625	Pa×s	571.95	Joback Method

dvisc	0.0000356	Pa×s	613.61	Joback Method
dvisc	0.0000218	Pa×s	655.28	Joback Method
dvisc	0.0000141	Pa×s	696.94	Joback Method
dvisc	0.0000096	Pa×s	738.61	Joback Method
dvisc	0.0000068	Pa×s	780.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R283588&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

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

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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume