Benzoic acid, 3-hydroxy-, tert.-butyl ester

Inchi: InChI=1S/C11H14O3/c1-11(2,3)14-10(13)8-5-4-6-9(12)7-8/h4-7,12H,1-3H3
InchiKey: XAOVNTXDHGDNBG-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(C)(C)OC(=O)c1cccc(O)c1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-231.55	kJ/mol	Joback Method
hf	-464.70	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.347		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
tb	631.44	K	Joback Method
tc	864.06	K	Joback Method
tf	426.45	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.94	J/mol×K	631.44	Joback Method
cpg	415.36	J/mol×K	670.21	Joback Method
cpg	427.79	J/mol×K	708.98	Joback Method
cpg	439.34	J/mol×K	747.75	Joback Method
cpg	450.09	J/mol×K	786.52	Joback Method
cpg	460.16	J/mol×K	825.29	Joback Method
cpg	469.65	J/mol×K	864.06	Joback Method
dvisc	0.0007018	Pa×s	426.45	Joback Method

dvisc	0.0003208	Pa×s	460.62	Joback Method
dvisc	0.0001634	Pa×s	494.78	Joback Method
dvisc	0.0000908	Pa×s	528.95	Joback Method
dvisc	0.0000542	Pa×s	563.11	Joback Method
dvisc	0.0000343	Pa×s	597.28	Joback Method
dvisc	0.0000228	Pa×s	631.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375415&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

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