Benzoic acid, 3-hydroxy-, 2-methylpropyl ester

Inchi: InChI=1S/C11H14O3/c1-8(2)7-14-11(13)9-4-3-5-10(12)6-9/h3-6,8,12H,7H2,1-2H3
InchiKey: WONJXDOZKTVJIO-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(C)COC(=O)c1cccc(O)c1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-236.83	kJ/mol	Joback Method
hf	-461.23	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.205		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1673.00		NIST Webbook
tb	634.23	K	Joback Method
tc	858.14	K	Joback Method
tf	409.03	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.03	J/mol×K	634.23	Joback Method
cpg	412.17	J/mol×K	671.55	Joback Method
cpg	424.47	J/mol×K	708.87	Joback Method
cpg	435.99	J/mol×K	746.18	Joback Method
cpg	446.79	J/mol×K	783.50	Joback Method
cpg	456.95	J/mol×K	820.82	Joback Method
cpg	466.52	J/mol×K	858.14	Joback Method
dvisc	0.0009998	Pa×s	409.03	Joback Method
dvisc	0.0004133	Pa×s	446.56	Joback Method

dvisc	0.0001960	Pa×s	484.10	Joback Method
dvisc	0.0001034	Pa×s	521.63	Joback Method
dvisc	0.0000595	Pa×s	559.16	Joback Method
dvisc	0.0000367	Pa×s	596.70	Joback Method
dvisc	0.0000240	Pa×s	634.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375425&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