Benzoic acid, 3-hydroxy-butyl ester

Inchi: InChI=1S/C11H14O3/c1-9(12)7-8-14-11(13)10-5-3-2-4-6-10/h2-6,9,12H,7-8H2,1H3
InchiKey: ZLYDSUAKIPQLNA-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(O)CCOC(=O)c1ccccc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-219.03	kJ/mol	Joback Method
hf	-436.15	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hvap	67.80	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.614		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1549.00		NIST Webbook
tb	645.79	K	Joback Method
tc	845.38	K	Joback Method
tf	358.13	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.54	J/mol×K	645.79	Joback Method
cpg	412.60	J/mol×K	679.05	Joback Method
cpg	423.95	J/mol×K	712.32	Joback Method
cpg	434.60	J/mol×K	745.58	Joback Method
cpg	444.56	J/mol×K	778.85	Joback Method
cpg	453.87	J/mol×K	812.11	Joback Method
cpg	462.54	J/mol×K	845.38	Joback Method
dvisc	0.0042275	Pa×s	358.13	Joback Method
dvisc	0.0013311	Pa×s	406.07	Joback Method

dvisc	0.0005350	Pa×s	454.02	Joback Method
dvisc	0.0002559	Pa×s	501.96	Joback Method
dvisc	0.0001392	Pa×s	549.90	Joback Method
dvisc	0.0000835	Pa×s	597.85	Joback Method
dvisc	0.0000540	Pa×s	645.79	Joback Method

Sources

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=U194380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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