Benzoic acid, 3-hydroxypropyl ester

Inchi: InChI=1S/C10H12O3/c11-7-4-8-13-10(12)9-5-2-1-3-6-9/h1-3,5-6,11H,4,7-8H2
InchiKey: BZISNWGGPWSXTK-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: O=C(OCCCO)c1ccccc1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-225.01	kJ/mol	Joback Method
hf	-410.23	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.226		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	623.35	K	Joback Method
tc	821.89	K	Joback Method
tf	361.86	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.28	J/mol×K	623.35	Joback Method
cpg	400.65	J/mol×K	788.80	Joback Method
cpg	392.00	J/mol×K	755.71	Joback Method
cpg	382.76	J/mol×K	722.62	Joback Method
cpg	372.90	J/mol×K	689.53	Joback Method
cpg	362.42	J/mol×K	656.44	Joback Method
cpg	408.71	J/mol×K	821.89	Joback Method
dvisc	0.0000688	Pa×s	623.35	Joback Method

dvisc	0.0001033	Pa×s	579.77	Joback Method
dvisc	0.0001658	Pa×s	536.19	Joback Method
dvisc	0.0002893	Pa×s	492.61	Joback Method
dvisc	0.0005624	Pa×s	449.02	Joback Method
dvisc	0.0012611	Pa×s	405.44	Joback Method
dvisc	0.0034351	Pa×s	361.86	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=R323116&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume