Benzoic acid, 4-tert-butyl-, propyl ester

Inchi: InChI=1S/C14H20O2/c1-5-10-16-13(15)11-6-8-12(9-7-11)14(2,3)4/h6-9H,5,10H2,1-4H3
InchiKey: IFFIRJMHMXRNHD-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	-61.30	kJ/mol	Joback Method
hf	-360.78	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.551		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
tb	624.44	K	Joback Method
tc	836.64	K	Joback Method
tf	361.06	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.87	J/mol×K	624.44	Joback Method
cpg	571.26	J/mol×K	801.27	Joback Method
cpg	558.30	J/mol×K	765.90	Joback Method
cpg	544.43	J/mol×K	730.54	Joback Method
cpg	529.60	J/mol×K	695.17	Joback Method
cpg	513.76	J/mol×K	659.81	Joback Method
cpg	583.33	J/mol×K	836.64	Joback Method
dvisc	0.0001311	Pa×s	624.44	Joback Method

dvisc	0.0001716	Pa×s	580.54	Joback Method
dvisc	0.0002346	Pa×s	536.65	Joback Method
dvisc	0.0003391	Pa×s	492.75	Joback Method
dvisc	0.0005268	Pa×s	448.85	Joback Method
dvisc	0.0009004	Pa×s	404.96	Joback Method
dvisc	0.0017532	Pa×s	361.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406138&Units=SI

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