Benzoic acid, 3-(1-methylpropyl)oxy-, methyl ester

Inchi: InChI=1S/C12H16O3/c1-4-9(2)15-11-7-5-6-10(8-11)12(13)14-3/h5-9H,4H2,1-3H3
InchiKey: YASTXHCEROOPQW-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: CCC(C)Oc1cccc(C(=O)OC)c1
Mol. weight [g/mol]: 208.25

Physical Properties

Property code	Value	Unit	Source
gf	-188.42	kJ/mol	Joback Method
hf	-448.25	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.651		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1544.00		NIST Webbook
tb	603.89	K	Joback Method
tc	812.91	K	Joback Method
tf	343.33	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.73	J/mol×K	603.89	Joback Method
cpg	434.72	J/mol×K	638.73	Joback Method
cpg	448.90	J/mol×K	673.56	Joback Method
cpg	462.28	J/mol×K	708.40	Joback Method
cpg	474.87	J/mol×K	743.24	Joback Method
cpg	486.66	J/mol×K	778.07	Joback Method
cpg	497.67	J/mol×K	812.91	Joback Method
dvisc	0.0015703	Pa×s	343.33	Joback Method
dvisc	0.0008297	Pa×s	386.76	Joback Method

dvisc	0.0004986	Pa×s	430.18	Joback Method
dvisc	0.0003290	Pa×s	473.61	Joback Method
dvisc	0.0002328	Pa×s	517.04	Joback Method
dvisc	0.0001738	Pa×s	560.46	Joback Method
dvisc	0.0001353	Pa×s	603.89	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=U375322&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