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

Inchi: InChI=1S/C15H22O3/c1-5-11(3)17-14-9-7-8-13(10-14)15(16)18-12(4)6-2/h7-12H,5-6H2,

InchiKey: JCGDBWWJKRWEPF-UHFFFAOYSA-N

Formula: C15H22O3

SMILES: CCC(C)OC(=O)c1cccc(OC(C)CC)c1

Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-165.60	kJ/mol	Joback Method
hf	-515.45	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.819		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook
tb	672.09	K	Joback Method
tc	875.92	K	Joback Method
tf	362.14	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.95	J/mol×K	672.09	Joback Method
cpg	591.84	J/mol×K	706.06	Joback Method
cpg	607.76	J/mol×K	740.03	Joback Method
cpg	622.73	J/mol×K	774.00	Joback Method
cpg	636.74	J/mol×K	807.97	Joback Method
cpg	649.82	J/mol×K	841.94	Joback Method
cpg	661.98	J/mol×K	875.92	Joback Method
dvisc	0.0016383	Pa×s	362.14	Joback Method

dvisc	0.0007488	Pa×s	413.80	Joback Method
dvisc	0.0004072	Pa×s	465.46	Joback Method
dvisc	0.0002501	Pa×s	517.12	Joback Method
dvisc	0.0001679	Pa×s	568.77	Joback Method
dvisc	0.0001204	Pa×s	620.43	Joback Method
dvisc	0.0000909	Pa×s	672.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375420&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