Benzoic acid, 3-isopropyloxy-, isopropyl ester

Inchi: InChI=1S/C13H18O3/c1-9(2)15-12-7-5-6-11(8-12)13(14)16-10(3)4/h5-10H,1-4H3
InchiKey: GZENFWQRRRRMGR-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CC(C)OC(=O)c1cccc(OC(C)C)c1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-182.44	kJ/mol	Joback Method
hf	-474.17	kJ/mol	Joback Method
hfus	20.01	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.039		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1542.00		NIST Webbook
tb	626.33	K	Joback Method
tc	836.17	K	Joback Method
tf	339.60	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.30	J/mol×K	626.33	Joback Method
cpg	486.26	J/mol×K	661.30	Joback Method
cpg	501.32	J/mol×K	696.28	Joback Method
cpg	515.49	J/mol×K	731.25	Joback Method
cpg	528.79	J/mol×K	766.22	Joback Method
cpg	541.21	J/mol×K	801.19	Joback Method
cpg	552.77	J/mol×K	836.17	Joback Method
dvisc	0.0018861	Pa×s	339.60	Joback Method
dvisc	0.0008851	Pa×s	387.39	Joback Method

dvisc	0.0004904	Pa×s	435.18	Joback Method
dvisc	0.0003054	Pa×s	482.96	Joback Method
dvisc	0.0002072	Pa×s	530.75	Joback Method
dvisc	0.0001498	Pa×s	578.54	Joback Method
dvisc	0.0001138	Pa×s	626.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375422&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