Benzenepropanoic acid 1-methylethyl ester

Other names:	3-Phenyl-propionic acid, isopropyl ester
	Isopropyl 3-phenylpropanoate
Inchi:	InChI=1S/C12H16O2/c1-10(2)14-12(13)9-8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey:	YQPAOLMOGAHRLG-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	22767-95-9

Physical Properties

Property code	Value	Unit	Source
gf	-73.79	kJ/mol	Joback Method
hf	-304.56	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.571		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1385.00		NIST Webbook
tb	576.49	K	Joback Method
tc	786.80	K	Joback Method
tf	308.58	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.41	J/mol×K	576.49	Joback Method
cpg	463.49	J/mol×K	751.74	Joback Method
cpg	451.37	J/mol×K	716.69	Joback Method
cpg	438.42	J/mol×K	681.64	Joback Method
cpg	424.63	J/mol×K	646.59	Joback Method
cpg	409.96	J/mol×K	611.54	Joback Method

cpg	474.82	J/mol×K	786.80	Joback Method
dvisc	0.0001725	Pa×s	576.49	Joback Method
dvisc	0.0002268	Pa×s	531.84	Joback Method
dvisc	0.0003136	Pa×s	487.19	Joback Method
dvisc	0.0004628	Pa×s	442.54	Joback Method
dvisc	0.0007455	Pa×s	397.88	Joback Method
dvisc	0.0013546	Pa×s	353.23	Joback Method
dvisc	0.0029260	Pa×s	308.58	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=C22767959&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

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