3-(4-isopropoxy-phenyl)-2-methyl-propionic acid, methyl ester

Inchi: InChI=1S/C14H20O3/c1-10(2)17-13-7-5-12(6-8-13)9-11(3)14(15)16-4/h5-8,10-11H,9H2,1

InchiKey: QYGNVPMXGZFFQB-UHFFFAOYSA-N

Formula: C14H20O3

SMILES: COC(=O)C(C)Cc1ccc(OC(C)C)cc1

Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-174.02	kJ/mol	Joback Method
hf	-494.81	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	60.49	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.825		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1565.30		NIST Webbook
rinpol	1565.30		NIST Webbook
tb	649.21	K	Joback Method
tc	855.88	K	Joback Method
tf	350.87	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.93	J/mol×K	649.21	Joback Method
cpg	595.02	J/mol×K	821.43	Joback Method
cpg	582.23	J/mol×K	786.99	Joback Method
cpg	568.54	J/mol×K	752.54	Joback Method
cpg	553.93	J/mol×K	718.10	Joback Method
cpg	538.40	J/mol×K	683.65	Joback Method
cpg	606.91	J/mol×K	855.88	Joback Method
dvisc	0.0001020	Pa×s	649.21	Joback Method

dvisc	0.0001347	Pa×s	599.49	Joback Method
dvisc	0.0001870	Pa×s	549.76	Joback Method
dvisc	0.0002773	Pa×s	500.04	Joback Method
dvisc	0.0004484	Pa×s	450.32	Joback Method
dvisc	0.0008171	Pa×s	400.59	Joback Method
dvisc	0.0017648	Pa×s	350.87	Joback Method

Sources

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=R157934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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