Phenylacetic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H18O3/c1-13(2)19-15-10-6-7-11-16(15)20-17(18)12-14-8-4-3-5-9-14/h3-11
InchiKey: BQBVAVUPDGTGNP-UHFFFAOYSA-N
Formula: C17H18O3
SMILES: CC(C)Oc1ccccc1OC(=O)Cc1ccccc1
Mol. weight [g/mol]: 270.32

Physical Properties

Property code	Value	Unit	Source
gf	-33.91	kJ/mol	Joback Method
hf	-314.92	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.622		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	744.97	K	Joback Method
tc	975.62	K	Joback Method
tf	426.10	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.97	J/mol×K	744.97	Joback Method
cpg	666.96	J/mol×K	937.18	Joback Method
cpg	655.76	J/mol×K	898.74	Joback Method
cpg	643.39	J/mol×K	860.30	Joback Method
cpg	629.83	J/mol×K	821.85	Joback Method
cpg	615.03	J/mol×K	783.41	Joback Method
cpg	677.03	J/mol×K	975.62	Joback Method
dvisc	0.0000778	Pa×s	744.97	Joback Method

dvisc	0.0001002	Pa×s	691.83	Joback Method
dvisc	0.0001347	Pa×s	638.68	Joback Method
dvisc	0.0001909	Pa×s	585.54	Joback Method
dvisc	0.0002901	Pa×s	532.39	Joback Method
dvisc	0.0004838	Pa×s	479.25	Joback Method
dvisc	0.0009165	Pa×s	426.10	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=U299007&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