3-Phenylpropionic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C18H20O3/c1-14(2)20-16-10-6-7-11-17(16)21-18(19)13-12-15-8-4-3-5-9-15/h3

InchiKey: FMOBBROVBXLZKT-UHFFFAOYSA-N

Formula: C18H20O3

SMILES: CC(C)Oc1ccccc1OC(=O)CCc1ccccc1

Mol. weight [g/mol]: 284.35

Physical Properties

Property code	Value	Unit	Source
gf	-25.49	kJ/mol	Joback Method
hf	-335.56	kJ/mol	Joback Method
hfus	30.52	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.012		Crippen Method
mcvol	230.270	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2083.00		NIST Webbook
tb	767.85	K	Joback Method
tc	994.69	K	Joback Method
tf	437.37	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.03	J/mol×K	767.85	Joback Method
cpg	670.29	J/mol×K	805.66	Joback Method
cpg	685.26	J/mol×K	843.46	Joback Method
cpg	699.00	J/mol×K	881.27	Joback Method
cpg	711.52	J/mol×K	919.08	Joback Method
cpg	722.87	J/mol×K	956.89	Joback Method
cpg	733.09	J/mol×K	994.69	Joback Method
dvisc	0.0008447	Pa×s	437.37	Joback Method
dvisc	0.0004401	Pa×s	492.45	Joback Method

dvisc	0.0002615	Pa×s	547.53	Joback Method
dvisc	0.0001709	Pa×s	602.61	Joback Method
dvisc	0.0001199	Pa×s	657.69	Joback Method
dvisc	0.0000889	Pa×s	712.77	Joback Method
dvisc	0.0000688	Pa×s	767.85	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=U299024&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