p-Toluic acid, 2-isopropoxyphenyl ester

Other names: p-Toluylic acid, 2-isopropoxyphenyl ester
Inchi: InChI=1S/C17H18O3/c1-12(2)19-15-6-4-5-7-16(15)20-17(18)14-10-8-13(3)9-11-14/h4-12
InchiKey: OORVOCNTIXBHBB-UHFFFAOYSA-N
Formula: C17H18O3
SMILES: Cc1ccc(C(=O)Oc2ccccc2OC(C)C)cc1
Mol. weight [g/mol]: 270.32

Physical Properties

Property code	Value	Unit	Source
gf	-43.54	kJ/mol	Joback Method
hf	-326.39	kJ/mol	Joback Method
hfus	27.54	kJ/mol	Joback Method
hvap	70.49	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.001		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1925.90		NIST Webbook
rinpol	1925.90		NIST Webbook
tb	749.95	K	Joback Method
tc	981.38	K	Joback Method
tf	438.62	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.01	J/mol×K	749.95	Joback Method
cpg	665.45	J/mol×K	942.81	Joback Method
cpg	654.35	J/mol×K	904.23	Joback Method
cpg	642.09	J/mol×K	865.66	Joback Method
cpg	628.62	J/mol×K	827.09	Joback Method
cpg	613.94	J/mol×K	788.52	Joback Method
cpg	675.40	J/mol×K	981.38	Joback Method

dvisc	0.0000781	Pa×s	749.95	Joback Method
dvisc	0.0000991	Pa×s	698.06	Joback Method
dvisc	0.0001307	Pa×s	646.17	Joback Method
dvisc	0.0001809	Pa×s	594.28	Joback Method
dvisc	0.0002663	Pa×s	542.40	Joback Method
dvisc	0.0004256	Pa×s	490.51	Joback Method
dvisc	0.0007599	Pa×s	438.62	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=U292645&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