p-Methoxybenzoic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H18O4/c1-12(2)20-15-6-4-5-7-16(15)21-17(18)13-8-10-14(19-3)11-9-13/h4

InchiKey: DRNGISTZXRQVQW-UHFFFAOYSA-N

Formula: C17H18O4

SMILES: COc1ccc(C(=O)Oc2ccccc2OC(C)C)cc1

Mol. weight [g/mol]: 286.32

Physical Properties

Property code	Value	Unit	Source
gf	-148.54	kJ/mol	Joback Method
hf	-458.61	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.702		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	2200.30		NIST Webbook
rinpol	2200.30		NIST Webbook
tb	772.37	K	Joback Method
tc	1000.99	K	Joback Method
tf	460.85	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.08	J/mol×K	772.37	Joback Method
cpg	689.41	J/mol×K	962.89	Joback Method
cpg	679.05	J/mol×K	924.78	Joback Method
cpg	667.44	J/mol×K	886.68	Joback Method
cpg	654.59	J/mol×K	848.58	Joback Method
cpg	640.47	J/mol×K	810.47	Joback Method
cpg	698.52	J/mol×K	1000.99	Joback Method
dvisc	0.0000600	Pa×s	772.37	Joback Method

dvisc	0.0000760	Pa×s	720.45	Joback Method
dvisc	0.0000998	Pa×s	668.53	Joback Method
dvisc	0.0001371	Pa×s	616.61	Joback Method
dvisc	0.0001998	Pa×s	564.69	Joback Method
dvisc	0.0003143	Pa×s	512.77	Joback Method
dvisc	0.0005475	Pa×s	460.85	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=U292652&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