

o-Methoxybenzoic acid, 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C17H18O4/c1-12(2)20-15-10-6-7-11-16(15)21-17(18)13-8-4-5-9-14(13)19-3/h
InchiKey:	NTBIEWQOLXLOLY-UHFFFAOYSA-N
Formula:	C17H18O4
SMILES:	COc1ccccc1C(=O)Oc1ccccc1OC(C)C
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	1977.50		NIST Webbook
rinpol	1977.50		NIST Webbook
tb	772.37	K	Joback Method
tc	1000.99	K	Joback Method
tf	460.85	K	Joback Method
vc	0.826	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.08	J/molxK	772.37	Joback Method
cpg	640.47	J/molxK	810.47	Joback Method
cpg	654.59	J/molxK	848.58	Joback Method
cpg	667.44	J/molxK	886.68	Joback Method
cpg	679.05	J/molxK	924.78	Joback Method
cpg	689.41	J/molxK	962.89	Joback Method
cpg	698.52	J/molxK	1000.99	Joback Method
dvisc	0.0005475	Paxs	460.85	Joback Method

dvisc	0.0003143	Paxs	512.77	Joback Method
dvisc	0.0001998	Paxs	564.69	Joback Method
dvisc	0.0001371	Paxs	616.61	Joback Method
dvisc	0.0000998	Paxs	668.53	Joback Method
dvisc	0.0000760	Paxs	720.45	Joback Method
dvisc	0.0000600	Paxs	772.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292619&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.chemeo.com/cid/90-162-2/o-Methoxybenzoic-acid-2-isopropoxyphenyl-ester.pdf>

Generated by Cheméo on 2024-04-26 22:14:53.316875439 +0000 UTC m=+16458942.237452758.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.