3-Isopropoxybenzoic acid, methyl ester

Other names:	Benzoic acid, 3-(isopropyl)oxy-, methyl ester
	Methyl 3-isopropoxybenzoate
Inchi:	InChI=1S/C11H14O3/c1-8(2)14-10-6-4-5-9(7-10)11(12)13-3/h4-8H,1-3H3
InchiKey:	GKWWRXCPQAQURQ-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	COC(=O)c1cccc(OC(C)C)c1
Mol. weight [g/mol]:	194.23
CAS:	350989-42-3

Physical Properties

Property code	Value	Unit	Source
gf	-196.84	kJ/mol	Joback Method
hf	-427.61	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.260		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1449.00		NIST Webbook
tb	581.01	K	Joback Method
tc	793.47	K	Joback Method
tf	332.06	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.20	J/mol×K	581.01	Joback Method
cpg	434.96	J/mol×K	758.06	Joback Method
cpg	423.70	J/mol×K	722.65	Joback Method
cpg	411.70	J/mol×K	687.24	Joback Method
cpg	398.95	J/mol×K	651.83	Joback Method
cpg	385.45	J/mol×K	616.42	Joback Method

cpg	445.46	J/mol×K	793.47	Joback Method
dvisc	0.0001487	Pa×s	581.01	Joback Method
dvisc	0.0001901	Pa×s	539.52	Joback Method
dvisc	0.0002532	Pa×s	498.03	Joback Method
dvisc	0.0003554	Pa×s	456.53	Joback Method
dvisc	0.0005336	Pa×s	415.04	Joback Method
dvisc	0.0008770	Pa×s	373.55	Joback Method
dvisc	0.0016320	Pa×s	332.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C350989423&Units=SI
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

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

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