Formic acid, 2-isopropylphenyl ester

Inchi: InChI=1S/C10H12O2/c1-8(2)9-5-3-4-6-10(9)12-7-11/h3-8H,1-2H3
InchiKey: QGWKAZQXXUFCQI-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(C)c1ccccc1OC=O
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-70.86	kJ/mol	Joback Method
hf	-247.75	kJ/mol	Joback Method
hfus	15.26	kJ/mol	Joback Method
hvap	49.53	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.345		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1211.00		NIST Webbook
tb	530.50	K	Joback Method
tc	743.78	K	Joback Method
tf	290.63	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.68	J/mol×K	530.50	Joback Method
cpg	314.96	J/mol×K	566.05	Joback Method
cpg	327.52	J/mol×K	601.59	Joback Method
cpg	339.37	J/mol×K	637.14	Joback Method
cpg	350.54	J/mol×K	672.68	Joback Method
cpg	361.04	J/mol×K	708.23	Joback Method
cpg	370.87	J/mol×K	743.78	Joback Method
dvisc	0.0025409	Pa×s	290.63	Joback Method

dvisc	0.0013130	Pa×s	330.61	Joback Method
dvisc	0.0007824	Pa×s	370.59	Joback Method
dvisc	0.0005156	Pa×s	410.56	Joback Method
dvisc	0.0003659	Pa×s	450.54	Joback Method
dvisc	0.0002746	Pa×s	490.52	Joback Method
dvisc	0.0002152	Pa×s	530.50	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=U368958&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