Formic acid, 2-propylphenyl ester

Inchi: InChI=1S/C10H12O2/c1-2-5-9-6-3-4-7-10(9)12-8-11/h3-4,6-8H,2,5H2,1H3
InchiKey: KWSAMNKWMADWHG-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CCCc1ccccc1OC=O
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-68.42	kJ/mol	Joback Method
hf	-242.47	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hvap	49.92	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.174		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
tb	530.94	K	Joback Method
tc	739.58	K	Joback Method
tf	305.63	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.37	J/mol×K	530.94	Joback Method
cpg	314.28	J/mol×K	565.71	Joback Method
cpg	326.52	J/mol×K	600.49	Joback Method
cpg	338.10	J/mol×K	635.26	Joback Method
cpg	349.03	J/mol×K	670.03	Joback Method
cpg	359.33	J/mol×K	704.80	Joback Method
cpg	369.00	J/mol×K	739.58	Joback Method
dvisc	0.0019637	Pa×s	305.63	Joback Method

dvisc	0.0011278	Pa×s	343.18	Joback Method
dvisc	0.0007226	Pa×s	380.73	Joback Method
dvisc	0.0005015	Pa×s	418.29	Joback Method
dvisc	0.0003697	Pa×s	455.84	Joback Method
dvisc	0.0002854	Pa×s	493.39	Joback Method
dvisc	0.0002286	Pa×s	530.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368966&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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