Formic acid, 1-phenylpropyl ester

Inchi: InChI=1S/C10H12O2/c1-2-10(12-8-11)9-6-4-3-5-7-9/h3-8,10H,2H2,1H3
InchiKey: BSYHSYBKNKZGNL-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CCC(OC=O)c1ccccc1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-61.23	kJ/mol	Joback Method
hf	-236.28	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	48.87	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.311		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1223.00		NIST Webbook
tb	525.52	K	Joback Method
tc	737.66	K	Joback Method
tf	278.11	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.83	J/mol×K	525.52	Joback Method
cpg	315.44	J/mol×K	560.88	Joback Method
cpg	328.28	J/mol×K	596.23	Joback Method
cpg	340.37	J/mol×K	631.59	Joback Method
cpg	351.72	J/mol×K	666.95	Joback Method
cpg	362.37	J/mol×K	702.31	Joback Method
cpg	372.32	J/mol×K	737.66	Joback Method
dvisc	0.0035559	Pa×s	278.11	Joback Method
dvisc	0.0016622	Pa×s	319.35	Joback Method

dvisc	0.0009245	Pa×s	360.58	Joback Method
dvisc	0.0005801	Pa×s	401.81	Joback Method
dvisc	0.0003969	Pa×s	443.05	Joback Method
dvisc	0.0002897	Pa×s	484.28	Joback Method
dvisc	0.0002222	Pa×s	525.52	Joback Method

Sources

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=U368962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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