Formic acid, 3-phenylpropyl ester

Inchi: InChI=1S/C10H12O2/c11-9-12-8-4-7-10-5-2-1-3-6-10/h1-3,5-6,9H,4,7-8H2
InchiKey: AMHRXSOVSAQOKL-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: O=COCCCc1ccccc1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-58.79	kJ/mol	Joback Method
hf	-231.00	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.792		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook
tb	525.96	K	Joback Method
tc	733.48	K	Joback Method
tf	293.11	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.53	J/mol×K	525.96	Joback Method
cpg	360.65	J/mol×K	698.89	Joback Method
cpg	350.21	J/mol×K	664.31	Joback Method
cpg	339.09	J/mol×K	629.72	Joback Method
cpg	327.29	J/mol×K	595.13	Joback Method
cpg	314.77	J/mol×K	560.55	Joback Method
cpg	370.44	J/mol×K	733.48	Joback Method
dvisc	0.0002358	Pa×s	525.96	Joback Method

dvisc	0.0003005	Pa×s	487.15	Joback Method
dvisc	0.0003993	Pa×s	448.34	Joback Method
dvisc	0.0005600	Pa×s	409.54	Joback Method
dvisc	0.0008430	Pa×s	370.73	Joback Method
dvisc	0.0013964	Pa×s	331.92	Joback Method
dvisc	0.0026437	Pa×s	293.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367887&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