

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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0009245	Paxs	360.58	Joback Method
dvisc	0.0005801	Paxs	401.81	Joback Method
dvisc	0.0003969	Paxs	443.05	Joback Method
dvisc	0.0002897	Paxs	484.28	Joback Method
dvisc	0.0002222	Paxs	525.52	Joback Method

Sources

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/ci9903071
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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