

Formic acid, 1-phenylethyl ester

Inchi:

InChI=1S/C9H10O2/c1-8(11-7-10)9-5-3-2-4-6-9/h2-8H,1H3

InchiKey:

RUDZCBIWUDOPTP-UHFFFAOYSA-N

Formula:

C9H10O2

SMILES:

CC(OC=O)c1ccccc1

Mol. weight [g/mol]:

150.17

Physical Properties

Property code	Value	Unit	Source
gf	-69.65	kJ/mol	Joback Method
hf	-215.64	kJ/mol	Joback Method
hfus	13.06	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.921		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1136.00		NIST Webbook
tb	502.64	K	Joback Method
tc	718.22	K	Joback Method
tf	266.84	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.99	J/mol×K	502.64	Joback Method
cpg	270.61	J/mol×K	538.57	Joback Method
cpg	282.51	J/mol×K	574.50	Joback Method
cpg	293.70	J/mol×K	610.43	Joback Method
cpg	304.22	J/mol×K	646.36	Joback Method
cpg	314.06	J/mol×K	682.29	Joback Method
cpg	323.26	J/mol×K	718.22	Joback Method
dvisc	0.0035759	Pa×s	266.84	Joback Method
dvisc	0.0017015	Pa×s	306.14	Joback Method

dvisc	0.0009586	Pa×s	345.44	Joback Method
dvisc	0.0006073	Pa×s	384.74	Joback Method
dvisc	0.0004187	Pa×s	424.04	Joback Method
dvisc	0.0003074	Pa×s	463.34	Joback Method
dvisc	0.0002369	Pa×s	502.64	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=U368941&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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