Formic acid phenyl ester

Other names: Phenyl formate
Inchi: InChI=1S/C7H6O2/c8-6-9-7-4-2-1-3-5-7/h1-6H
InchiKey: GEOWCLRLLWTHDN-UHFFFAOYSA-N
Formula: C7H6O2
SMILES: O=COc1ccccc1
Mol. weight [g/mol]: 122.12
CAS: 1864-94-4

Physical Properties

Property code	Value	Unit	Source
chl	-3343.40 ± 2.80	kJ/mol	NIST Webbook
gf	-84.05	kJ/mol	Joback Method
hf	-215.70 ± 3.10	kJ/mol	NIST Webbook
hfl	-268.60 ± 2.90	kJ/mol	NIST Webbook
hfus	11.40	kJ/mol	Joback Method
hvap	52.90 ± 0.60	kJ/mol	NIST Webbook
hvap	52.90	kJ/mol	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.222		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	457.32	K	Joback Method
tc	674.46	K	Joback Method
tf	259.30	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.11	J/mol×K	457.32	Joback Method
cpg	185.95	J/mol×K	493.51	Joback Method
cpg	195.24	J/mol×K	529.70	Joback Method
cpg	203.99	J/mol×K	565.89	Joback Method
cpg	212.22	J/mol×K	602.08	Joback Method

cpg	219.93	J/mol×K	638.27	Joback Method
cpg	227.13	J/mol×K	674.46	Joback Method
dvisc	0.0024487	Pa×s	259.30	Joback Method
dvisc	0.0013796	Pa×s	292.30	Joback Method
dvisc	0.0008732	Pa×s	325.31	Joback Method
dvisc	0.0006013	Pa×s	358.31	Joback Method
dvisc	0.0004409	Pa×s	391.31	Joback Method
dvisc	0.0003393	Pa×s	424.32	Joback Method
dvisc	0.0002712	Pa×s	457.32	Joback Method
hvapt	52.90 ± 1.00	kJ/mol	287.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1864944&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume