Formic acid, phenylmethyl ester

Other names:	Benzyl alcohol, formate
	Benzyl formate
	Benzyl methanoate
	Formic acid, benzyl ester
	Benzylester kyseliny mravenci
Inchi:	InChI=1S/C8H8O2/c9-7-10-6-8-4-2-1-3-5-8/h1-5,7H,6H2
InchiKey:	UYWQUFXKFGHYNT-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	O=COCc1ccccc1
Mol. weight [g/mol]:	136.15
CAS:	104-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-75.63	kJ/mol	Joback Method
hf	-189.72	kJ/mol	Joback Method
hfus	13.99	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.360		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1077.30		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1081.20		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1081.60		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook

rinpol	1046.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1081.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1673.00		NIST Webbook
tb	476.15 ± 0.40	K	NIST Webbook
tc	694.16	K	Joback Method
tf	270.57	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.88	J/mol×K	480.20	Joback Method
cpg	227.01	J/mol×K	515.86	Joback Method
cpg	237.52	J/mol×K	551.52	Joback Method
cpg	247.42	J/mol×K	587.18	Joback Method
cpg	256.74	J/mol×K	622.84	Joback Method
cpg	265.47	J/mol×K	658.50	Joback Method
cpg	273.65	J/mol×K	694.16	Joback Method
dvisc	0.0025641	Pa×s	270.57	Joback Method
dvisc	0.0014118	Pa×s	305.51	Joback Method
dvisc	0.0008786	Pa×s	340.45	Joback Method
dvisc	0.0005973	Pa×s	375.38	Joback Method
dvisc	0.0004336	Pa×s	410.32	Joback Method
dvisc	0.0003310	Pa×s	445.26	Joback Method
dvisc	0.0002628	Pa×s	480.20	Joback Method
hvapt	51.60	kJ/mol	327.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	1.30	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104574&Units=SI

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume