Formic acid, 2-phenylethyl ester

Other names:	Phenethyl alcohol, formate
	«beta»-Phenethyl formate
	«beta»-Phenylethyl formate
	Benzeneethanol, formate
	Benzylcarbinyl formate
	Phenethyl formate
	2-Phenethyl formate
	2-Phenylethyl formate
	Formic acid, phenethyl ester
	Phenylethyl formate
	2-Fenylethylester kyseliny mravenci
	NSC 404456
Inchi:	InChI=1S/C9H10O2/c10-8-11-7-6-9-4-2-1-3-5-9/h1-5,8H,6-7H2
InchiKey:	IKDIJXDZEYHZSD-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	O=COCCc1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	104-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-67.21	kJ/mol	Joback Method
hf	-210.36	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	47.03	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.402		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1141.90		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1138.50		NIST Webbook
rinpol	1156.00		NIST Webbook

rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
ripol	1778.70		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1768.00		NIST Webbook
tb	503.08	K	Joback Method
tc	713.81	K	Joback Method
tf	281.84	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.72	J/mol×K	503.08	Joback Method
cpg	312.40	J/mol×K	678.69	Joback Method
cpg	302.75	J/mol×K	643.57	Joback Method
cpg	292.48	J/mol×K	608.44	Joback Method
cpg	281.56	J/mol×K	573.32	Joback Method
cpg	269.98	J/mol×K	538.20	Joback Method
cpg	321.44	J/mol×K	713.81	Joback Method
dvisc	0.0002506	Pa×s	503.08	Joback Method
dvisc	0.0003176	Pa×s	466.21	Joback Method
dvisc	0.0004191	Pa×s	429.33	Joback Method
dvisc	0.0005827	Pa×s	392.46	Joback Method
dvisc	0.0008675	Pa×s	355.59	Joback Method
dvisc	0.0014161	Pa×s	318.71	Joback Method
dvisc	0.0026277	Pa×s	281.84	Joback Method

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=C104621&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume