

2-Propen-1-ol, 3-phenyl-, formate

Other names:	Cinnamyl alcohol, formate «gamma»-Phenylallyl formate Cinnamyl formate Cinnamyl methanoate Formic acid, cinnamyl ester 3-Phenyl-2-propen-1-yl formate
Inchi:	InChI=1S/C10H10O2/c11-9-12-8-4-7-10-5-2-1-3-6-10/h1-7,9H,8H2/b7-4+
InchiKey:	LBHJXKYRYCUGPD-QPJJXVBHSA-N
Formula:	C10H10O2
SMILES:	O=COCC=Cc1ccccc1
Mol. weight [g/mol]:	162.19
CAS:	104-65-4

Physical Properties

Property code	Value	Unit	Source
gf	21.43	kJ/mol	Joback Method
hf	-113.78	kJ/mol	Joback Method
hfus	19.38	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.873		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1330.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2094.00		NIST Webbook
tb	530.12	K	Joback Method
tc	747.33	K	Joback Method
tf	288.03	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.09	J/mol×K	530.12	Joback Method
cpg	295.79	J/mol×K	566.32	Joback Method
cpg	307.68	J/mol×K	602.52	Joback Method
cpg	318.81	J/mol×K	638.72	Joback Method
cpg	329.20	J/mol×K	674.93	Joback Method
cpg	338.89	J/mol×K	711.13	Joback Method
cpg	347.92	J/mol×K	747.33	Joback Method
dvisc	0.0024293	Pa×s	288.03	Joback Method
dvisc	0.0012400	Pa×s	328.38	Joback Method
dvisc	0.0007333	Pa×s	368.73	Joback Method
dvisc	0.0004810	Pa×s	409.08	Joback Method
dvisc	0.0003403	Pa×s	449.42	Joback Method
dvisc	0.0002549	Pa×s	489.77	Joback Method
dvisc	0.0001995	Pa×s	530.12	Joback Method

Sources

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=C104654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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