1,3-Benzodioxole-5-propanal, «alpha»-methyl-

Other names:	«alpha»-Methyl-3,4-methylenedioxy-hydrocinnamic aldehyde Hydrocinnamaldehyde, «alpha»-methyl-3,4-(methylenedioxy)- Helional «alpha»-methyl-1,3-benzodioxole-5-propionaldehyde
Inchi:	InChI=1S/C11H12O3/c1-8(6-12)4-9-2-3-10-11(5-9)14-7-13-10/h2-3,5-6,8H,4,7H2,1H3
InchiKey:	BOPPSUHPZARXTH-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	CC(C=O)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	192.21
CAS:	1205-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-70.85	kJ/mol	Joback Method
hf	-318.50	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.793		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1541.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	601.25	K	Joback Method
tc	825.96	K	Joback Method
tf	367.51	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.01	J/mol×K	601.25	Joback Method
cpg	377.10	J/mol×K	638.70	Joback Method
cpg	389.26	J/mol×K	676.15	Joback Method

cpg	400.57	J/mol×K	713.60	Joback Method
cpg	411.09	J/mol×K	751.06	Joback Method
cpg	420.89	J/mol×K	788.51	Joback Method
cpg	430.03	J/mol×K	825.96	Joback Method
dvisc	0.0028674	Pa×s	367.51	Joback Method
dvisc	0.0018439	Pa×s	406.47	Joback Method
dvisc	0.0012809	Pa×s	445.42	Joback Method
dvisc	0.0009435	Pa×s	484.38	Joback Method
dvisc	0.0007273	Pa×s	523.34	Joback Method
dvisc	0.0005813	Pa×s	562.29	Joback Method
dvisc	0.0004783	Pa×s	601.25	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=C1205170&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