

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	1543.00		NIST Webbook
rinpol	1541.00		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/molxK	601.25	Joback Method
cpg	420.89	J/molxK	788.51	Joback Method
cpg	411.09	J/molxK	751.06	Joback Method

cpg	400.57	J/molxK	713.60	Joback Method
cpg	389.26	J/molxK	676.15	Joback Method
cpg	377.10	J/molxK	638.70	Joback Method
cpg	430.03	J/molxK	825.96	Joback Method
dvisc	0.0004783	Paxs	601.25	Joback Method
dvisc	0.0005813	Paxs	562.29	Joback Method
dvisc	0.0007273	Paxs	523.34	Joback Method
dvisc	0.0009435	Paxs	484.38	Joback Method
dvisc	0.0012809	Paxs	445.42	Joback Method
dvisc	0.0018439	Paxs	406.47	Joback Method
dvisc	0.0028674	Paxs	367.51	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

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