Helional

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

Physical Properties

Property code	Value	Unit	Source
hfus	29.30	kJ/mol	Joback Method
hvap	70.93	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	1.793		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1541.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	543.25	K	Cheméo Relay (1.0)
tf	309.57	K	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1205170&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point