2«beta»-acetoxy-6«alpha»-methoxyformyl-trans-d

Inchi: InChI=1S/C14H22O4/c1-9(15)18-13-6-5-10-7-12(14(16)17-2)4-3-11(10)8-13/h10-13H,3-8
InchiKey: NCMSMIKABKRKAE-IFWUJCSASA-N
Formula: C14H22O4
SMILES: COC(=O)C1CCC2CC(OC(C)=O)CCC2C1
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-343.16	kJ/mol	Joback Method
hf	-741.61	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.308		Crippen Method
mcvol	201.280	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
ripol	2512.00		NIST Webbook
tb	693.52	K	Joback Method
tc	911.14	K	Joback Method
tf	405.18	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.68	J/mol×K	693.52	Joback Method
cpg	628.72	J/mol×K	729.79	Joback Method
cpg	647.41	J/mol×K	766.06	Joback Method
cpg	664.76	J/mol×K	802.33	Joback Method
cpg	680.80	J/mol×K	838.60	Joback Method
cpg	695.53	J/mol×K	874.87	Joback Method
cpg	708.98	J/mol×K	911.14	Joback Method

dvisc	0.0020657	Pa×s	405.18	Joback Method
dvisc	0.0013268	Pa×s	453.24	Joback Method
dvisc	0.0009277	Pa×s	501.29	Joback Method
dvisc	0.0006906	Pa×s	549.35	Joback Method
dvisc	0.0005390	Pa×s	597.41	Joback Method
dvisc	0.0004366	Pa×s	645.46	Joback Method
dvisc	0.0003641	Pa×s	693.52	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=R136140&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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