

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,3-8H
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/molxK	693.52	Joback Method
cpg	628.72	J/molxK	729.79	Joback Method
cpg	647.41	J/molxK	766.06	Joback Method
cpg	664.76	J/molxK	802.33	Joback Method
cpg	680.80	J/molxK	838.60	Joback Method
cpg	695.53	J/molxK	874.87	Joback Method
cpg	708.98	J/molxK	911.14	Joback Method

dvisc	0.0020657	Paxs	405.18	Joback Method
dvisc	0.0013268	Paxs	453.24	Joback Method
dvisc	0.0009277	Paxs	501.29	Joback Method
dvisc	0.0006906	Paxs	549.35	Joback Method
dvisc	0.0005390	Paxs	597.41	Joback Method
dvisc	0.0004366	Paxs	645.46	Joback Method
dvisc	0.0003641	Paxs	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/ci9903071

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
mvol:	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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