2«beta»-hydroxy-6«beta»-methoxyformyl-trans-de

Inchi: InChI=1S/C12H20O3/c1-15-12(14)10-3-2-9-7-11(13)5-4-8(9)6-10/h8-11,13H,2-7H2,1H3/
InchiKey: WDHAHCIDYFOARH-JPPWEJMLSA-N
Formula: C12H20O3
SMILES: COC(=O)C1CCC2CC(O)CCC2C1
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-262.90	kJ/mol	Joback Method
hf	-607.76	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	68.04	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.737		Crippen Method
mcvol	171.530	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1665.00		NIST Webbook
ripol	2656.00		NIST Webbook
tb	663.65	K	Joback Method
tc	869.13	K	Joback Method
tf	371.30	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.36	J/mol×K	663.65	Joback Method
cpg	532.14	J/mol×K	697.90	Joback Method
cpg	548.83	J/mol×K	732.14	Joback Method
cpg	564.45	J/mol×K	766.39	Joback Method
cpg	579.03	J/mol×K	800.63	Joback Method
cpg	592.60	J/mol×K	834.88	Joback Method
cpg	605.17	J/mol×K	869.13	Joback Method
dvisc	0.0042886	Pa×s	371.30	Joback Method

dvisc	0.0017578	Pa×s	420.02	Joback Method
dvisc	0.0008673	Pa×s	468.75	Joback Method
dvisc	0.0004888	Pa×s	517.48	Joback Method
dvisc	0.0003041	Pa×s	566.20	Joback Method
dvisc	0.0002039	Pa×s	614.92	Joback Method
dvisc	0.0001450	Pa×s	663.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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