

2«alpha»-acetoxy-6«alpha»-hydroxy-trans-decalin

Inchi:	InChI=1S/C12H20O3/c1-8(13)15-12-5-3-9-6-11(14)4-2-10(9)7-12/h9-12,14H,2-7H2,1H3/
InchiKey:	KGOAGXZCQFDBOX-QQFIATSDSA-N
Formula:	C12H20O3
SMILES:	CC(=O)OC1CCC2CC(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	-2.50		Crippen Method
logp	1.879		Crippen Method
mcvol	171.530	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpola	1613.00		NIST Webbook
ripola	2531.00		NIST Webbook
tb	663.65	K	Joback Method
tc	869.13	K	Joback Method
tf	371.30	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0017578	Paxs	420.02	Joback Method
dvisc	0.0008673	Paxs	468.75	Joback Method
dvisc	0.0004888	Paxs	517.48	Joback Method
dvisc	0.0003041	Paxs	566.20	Joback Method
dvisc	0.0002039	Paxs	614.92	Joback Method
dvisc	0.0001450	Paxs	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=R136006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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