4-«alpha»,4a-«alpha»,7-«alpha»,7a-«alpha»-Dihyd 3-hydroxy

InChI: InChI=1S/C10H16O3/c1-5-3-4-7-6(2)9(11)13-10(12)8(5)7/h5-9,11H,3-4H2,1-2H3/t5-,6+,7

InChIKey: PLWVFYKDQKCFIY-ICHFNJPQSA-N

Formula: C10H16O3

SMILES: CC1CCC2C(C)C(O)OC(=O)C12

Mol. weight [g/mol]: 184.23

Physical Properties

Property code	Value	Unit	Source
gf	-250.14	kJ/mol	Joback Method
hf	-605.56	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	62.70	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.160		Crippen Method
mcvol	143.350	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
tb	627.43	K	Joback Method
tc	838.04	K	Joback Method
tf	370.67	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.16	J/mol×K	627.43	Joback Method
cpg	442.13	J/mol×K	662.53	Joback Method
cpg	458.15	J/mol×K	697.63	Joback Method
cpg	473.22	J/mol×K	732.74	Joback Method
cpg	487.34	J/mol×K	767.84	Joback Method
cpg	500.52	J/mol×K	802.94	Joback Method
cpg	512.78	J/mol×K	838.04	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=R197145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume