

(6R)-7a-Hydroxy-3,6-dimethyl-5,6,7,7a-tetrahydrok

Inchi:	InChI=1S/C10H14O3/c1-6-3-4-8-7(2)9(11)13-10(8,12)5-6/h6,12H,3-5H2,1-2H3
InchiKey:	LBNWZGLSMCTAQB-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CC1=C2CCC(C)CC2(O)OC1=O
Mol. weight [g/mol]:	182.22
CAS:	213969-56-3

Physical Properties

Property code	Value	Unit	Source
gf	-221.80	kJ/mol	Joback Method
hf	-494.46	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	64.10	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.368		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1566.80		NIST Webbook
rinpol	1566.80		NIST Webbook
ripol	2900.00		NIST Webbook
ripol	2900.00		NIST Webbook
tb	650.80	K	Joback Method
tc	872.95	K	Joback Method
tf	433.09	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.05	J/molxK	650.80	Joback Method
cpg	405.94	J/molxK	687.83	Joback Method
cpg	419.16	J/molxK	724.85	Joback Method
cpg	431.83	J/molxK	761.88	Joback Method
cpg	444.05	J/molxK	798.90	Joback Method

cpg	455.94	J/mol×K	835.93	Joback Method
cpg	467.59	J/mol×K	872.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C213969563&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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