Senkyunolide H

Inchi: InChI=1S/C12H16O4/c1-2-3-4-9-7-5-6-8(13)11(14)10(7)12(15)16-9/h4,8,11,13-14H,2-3,5
InchiKey: DQNGMIQSXNGHOA-WTKPLQERSA-N
Formula: C12H16O4
SMILES: CCCC=C1OC(=O)C2=C1CCC(O)C2O
Mol. weight [g/mol]: 224.25
CAS: 94596-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-290.83	kJ/mol	Joback Method
hf	-627.18	kJ/mol	Joback Method
hfus	33.24	kJ/mol	Joback Method
hvap	87.17	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.039		Crippen Method
mcvol	168.800	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	2033.90		NIST Webbook
tb	795.14	K	Joback Method
tc	998.83	K	Joback Method
tf	502.91	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.94	J/mol×K	795.14	Joback Method
cpg	539.66	J/mol×K	829.09	Joback Method
cpg	550.64	J/mol×K	863.04	Joback Method
cpg	560.90	J/mol×K	896.99	Joback Method
cpg	570.47	J/mol×K	930.93	Joback Method
cpg	579.35	J/mol×K	964.88	Joback Method
cpg	587.59	J/mol×K	998.83	Joback Method

Sources

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=C94596277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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