Senkyunolide N

Inchi: InChI=1S/C12H18O4/c1-2-3-4-9-7-5-6-8(13)11(14)10(7)12(15)16-9/h8-9,11,13-14H,2-6H
InchiKey: AXRIHSJZHOTGAE-UHFFFAOYSA-N
Formula: C12H18O4
SMILES: CCCCC1OC(=O)C2=C1CCC(O)C2O
Mol. weight [g/mol]: 226.27
CAS: 140694-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-344.00	kJ/mol	Joback Method
hf	-723.55	kJ/mol	Joback Method
hfus	33.99	kJ/mol	Joback Method
hvap	86.07	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	0.914		Crippen Method
mcvol	173.100	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1985.80		NIST Webbook
tb	783.83	K	Joback Method
tc	983.26	K	Joback Method
tf	488.31	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.35	J/mol×K	783.83	Joback Method
cpg	572.19	J/mol×K	817.07	Joback Method
cpg	584.20	J/mol×K	850.31	Joback Method
cpg	595.41	J/mol×K	883.54	Joback Method
cpg	605.82	J/mol×K	916.78	Joback Method
cpg	615.46	J/mol×K	950.02	Joback Method
cpg	624.32	J/mol×K	983.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140694582&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
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