Senkyunolide P

Inchi: InChI=1S/C24H30O4/c1-3-5-7-18-16-10-9-15-14-11-12-24(21(15)20(16)23(26)27-18)17(
InchiKey: YTEUTQUNVHWZOR-WSVATBPTSA-N
Formula: C24H30O4
SMILES: CCCC=C1OC(=O)C2=C1CCC1C3C=C4C(=O)OC(CCCC)C4(CC3)C21
Mol. weight [g/mol]: 382.49
CAS: 142864-23-1

Physical Properties

Property code	Value	Unit	Source
gf	72.23	kJ/mol	Joback Method
hf	-560.15	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.002		Crippen Method
mcvol	296.700	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	2900.00		NIST Webbook
tb	1004.71	K	Joback Method
tc	1249.27	K	Joback Method
tf	702.30	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.28	J/mol×K	1004.71	Joback Method
cpg	1127.71	J/mol×K	1045.47	Joback Method
cpg	1152.47	J/mol×K	1086.23	Joback Method
cpg	1177.84	J/mol×K	1126.99	Joback Method
cpg	1204.08	J/mol×K	1167.75	Joback Method
cpg	1231.48	J/mol×K	1208.51	Joback Method
cpg	1260.30	J/mol×K	1249.27	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=C142864231&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