

Senkyunolide

Other names:	(S)-3-Butyl-4,5-dihydroisobenzofuran-1(3H)-one Sedanenolide (S)-Sedanenolide Senkyunolide A 3-n-Butyl-4,5-dihydrophthalide 1(3H)-Isobenzofuranone, 3-butyl-4,5-dihydro-, (-)- (-)-Sedanenolide 1(3H)-Isobenzofuranone, 3-butyl-4,5-dihydro-, (S)-
Inchi:	InChI=1S/C12H16O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h5,7,11H,2-4,6,8H2,1H3
InchiKey:	ZPIKVDODKLJKIN-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	<chem>CCCCC1OC(=O)C2=C1CCC=C2</chem>
Mol. weight [g/mol]:	192.25
CAS:	62006-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.98	kJ/mol	Joback Method
hf	-320.63	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.749		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1729.00		NIST Webbook
tb	607.97	K	Joback Method
tc	833.96	K	Joback Method
tf	375.91	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.73	J/molxK	607.97	Joback Method
cpg	431.80	J/molxK	645.64	Joback Method
cpg	447.84	J/molxK	683.30	Joback Method
cpg	462.88	J/molxK	720.97	Joback Method
cpg	476.96	J/molxK	758.63	Joback Method
cpg	490.11	J/molxK	796.30	Joback Method
cpg	502.36	J/molxK	833.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62006397&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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