sedanonic acid lactone

Other names: Z-butylidene-4,5,6,7-tetrahydrophthalide
Inchi: InChI=1S/C12H16O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h8H,2-7H2,1H3/b11-8-
InchiKey: YHOZXUUDDDOBKS-FLIBITNWSA-N
Formula: C12H16O2
SMILES: CCCC=C1OC(=O)C2=C1CCCC2
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-1.77	kJ/mol	Joback Method
hf	-282.04	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	54.43	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.098		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1711.00		NIST Webbook
tb	620.12	K	Joback Method
tc	850.84	K	Joback Method
tf	389.75	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.68	J/mol×K	620.12	Joback Method
cpg	429.33	J/mol×K	658.57	Joback Method
cpg	444.94	J/mol×K	697.03	Joback Method
cpg	459.57	J/mol×K	735.48	Joback Method
cpg	473.27	J/mol×K	773.93	Joback Method
cpg	486.07	J/mol×K	812.38	Joback Method
cpg	498.03	J/mol×K	850.84	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=U374194&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