sedanenolide

Inchi: InChI=1S/C12H16O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h7-9H,2-6H2,1H3/b11-8-
InchiKey: OFKAWRNOBJDJFC-FLIBITNWSA-N
Formula: C12H16O2
SMILES: CCCC=C1OC(=O)C2=CCCCC12
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	0.15	kJ/mol	Joback Method
hf	-290.91	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.954		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	610.47	K	Joback Method
tc	840.28	K	Joback Method
tf	372.99	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.04	J/mol×K	610.47	Joback Method
cpg	432.43	J/mol×K	648.77	Joback Method
cpg	448.74	J/mol×K	687.07	Joback Method
cpg	464.01	J/mol×K	725.38	Joback Method
cpg	478.29	J/mol×K	763.68	Joback Method
cpg	491.61	J/mol×K	801.98	Joback Method
cpg	504.02	J/mol×K	840.28	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=R219364&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