

(.+/-.)-Eldanolide

Inchi:	InChI=1S/C10H16O2/c1-7(2)4-5-9-8(3)6-10(11)12-9/h4,8-9H,5-6H2,1-3H3
InchiKey:	ARNPQYFYGKMXGD-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)=CCC1OC(=O)CC1C
Mol. weight [g/mol]:	168.23
CAS:	92843-42-0

Physical Properties

Property code	Value	Unit	Source
gf	-74.88	kJ/mol	Joback Method
hf	-371.86	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	46.60	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.294		Crippen Method
mvol	144.040	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	1421.50		NIST Webbook
rinpol	1421.50		NIST Webbook
tb	537.62	K	Joback Method
tc	755.33	K	Joback Method
tf	284.87	K	Joback Method
vc	0.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.84	J/molxK	537.62	Joback Method
cpg	370.38	J/molxK	573.91	Joback Method
cpg	387.04	J/molxK	610.19	Joback Method
cpg	402.80	J/molxK	646.48	Joback Method
cpg	417.70	J/molxK	682.76	Joback Method
cpg	431.75	J/molxK	719.05	Joback Method
cpg	444.95	J/molxK	755.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92843420&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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