ISOALANTOLACTONE

Other names: Eudesma-4(14),11(13)-dien-12-oic acid, 8-«beta»-hydroxy-, «gamma»-lactone
Isoalantolactone
Inchi: InChI=1S/C15H20O2/c1-9-5-4-6-15(3)8-13-11(7-12(9)15)10(2)14(16)17-13/h11-13H,1-2,
InchiKey: CVUANYCQTOGILD-UHFFFAOYSA-N
Formula: C15H20O2
SMILES: C=C1C(=O)OC2CC3(C)CCCC(=C)C3CC12
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
hfus	20.56	kJ/mol	Joback Method
logp	3.241		Crippen Method
mcvol	188.470	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.67	J/mol×K	668.56	Joback Method
cpg	580.06	J/mol×K	708.99	Joback Method
cpg	600.23	J/mol×K	749.43	Joback Method
cpg	619.34	J/mol×K	789.86	Joback Method
cpg	637.56	J/mol×K	830.29	Joback Method
cpg	655.08	J/mol×K	870.73	Joback Method
cpg	672.06	J/mol×K	911.16	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C470177&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume