Eudesma-4(15),7(11),8-trien-12-olide

Other names: Eudesma-4(15),7(11),9-trien-12-olide
Inchi: InChI=1S/C15H18O2/c1-9-5-4-6-15(3)8-13-11(7-12(9)15)10(2)14(16)17-13/h8,12H,1,4-7
InchiKey: ZTVSGQPHMUYCRS-CVRLYYSRSA-N
Formula: C15H18O2
SMILES: C=C1CCCC2(C)C=C3OC(=O)C(C)=C3CC12
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	86.89	kJ/mol	Joback Method
hf	-227.90	kJ/mol	Joback Method
hfus	20.85	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.510		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1968.00		NIST Webbook
tb	692.00	K	Joback Method
tc	939.30	K	Joback Method
tf	474.24	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.04	J/mol×K	692.00	Joback Method
cpg	548.73	J/mol×K	733.22	Joback Method
cpg	566.46	J/mol×K	774.43	Joback Method
cpg	583.44	J/mol×K	815.65	Joback Method
cpg	599.86	J/mol×K	856.87	Joback Method
cpg	615.91	J/mol×K	898.09	Joback Method
cpg	631.77	J/mol×K	939.30	Joback Method

Sources

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=R424130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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