1,10-seco-Eudesma-4(15),5(10)-dien-1-al

Inchi: InChI=1S/C15H24O/c1-11(2)14-8-7-13(4)15(10-14)12(3)6-5-9-16/h9,11,14H,3,5-8,10H2,
InchiKey: PKMQICXYDJHITQ-UHFFFAOYSA-N
Formula: C15H24O
SMILES: C=C(CCC=O)C1=C(C)CCC(C(C)C)C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	87.90	kJ/mol	Joback Method
hf	-238.99	kJ/mol	Joback Method
hfus	23.06	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.294		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1574.00		NIST Webbook
tb	616.05	K	Joback Method
tc	819.07	K	Joback Method
tf	303.27	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.04	J/mol×K	616.05	Joback Method
cpg	560.24	J/mol×K	649.89	Joback Method
cpg	578.39	J/mol×K	683.72	Joback Method
cpg	595.52	J/mol×K	717.56	Joback Method
cpg	611.66	J/mol×K	751.39	Joback Method
cpg	626.86	J/mol×K	785.23	Joback Method
cpg	641.14	J/mol×K	819.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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