

1 «beta»-acetoxyfurano-4(15)-eudesmene

Inchi:	InChI=1S/C17H24O3/c1-10-5-6-16(20-12(3)18)17(4)8-15-13(7-14(10)17)11(2)9-19-15/h
InchiKey:	OXDNGGSXVJGGNR-PPRXNKMGSA-N
Formula:	C17H24O3
SMILES:	<chem>C=C1CCC(OC(C)=O)C2(C)CC3OC=C(C)C3CC12</chem>
Mol. weight [g/mol]:	276.37

Physical Properties

Property code	Value	Unit	Source
gf	-41.43	kJ/mol	Joback Method
hf	-472.14	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.603		Crippen Method
mvol	222.520	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
ripol	2723.00		NIST Webbook
ripol	2723.00		NIST Webbook
tb	723.10	K	Joback Method
tc	949.18	K	Joback Method
tf	462.20	K	Joback Method
vc	0.838	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.83	J/mol×K	723.10	Joback Method
cpg	709.66	J/mol×K	760.78	Joback Method
cpg	729.45	J/mol×K	798.46	Joback Method
cpg	748.35	J/mol×K	836.14	Joback Method
cpg	766.53	J/mol×K	873.82	Joback Method
cpg	784.14	J/mol×K	911.50	Joback Method
cpg	801.33	J/mol×K	949.18	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=R395423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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