

labda-13-(E)-en-8«alpha»-15yl acetate

Inchi:	InChI=1S/C24H40O4/c1-17(12-16-27-18(2)25)9-10-21-23(6)14-8-13-22(4,5)20(23)11-15
InchiKey:	LDRJQXFQGSRDEB-IUBNAXQHSA-N
Formula:	C24H40O4
SMILES:	CC(=O)OCC=C(C)CCC1C(C)(OC(C)=O)CCC2C(C)(C)CCCC21C
Mol. weight [g/mol]:	392.57

Physical Properties

Property code	Value	Unit	Source
gf	-211.47	kJ/mol	Joback Method
hf	-815.20	kJ/mol	Joback Method
hfus	34.57	kJ/mol	Joback Method
hvap	83.50	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.840		Crippen Method
mcvol	337.880	ml/mol	McGowan Method
pc	1128.35	kPa	Joback Method
rinsol	2505.00		NIST Webbook
tb	922.41	K	Joback Method
tc	1145.01	K	Joback Method
tf	566.30	K	Joback Method
vc	1.282	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.00	J/mol×K	922.41	Joback Method
cpg	1216.75	J/mol×K	959.51	Joback Method
cpg	1247.40	J/mol×K	996.61	Joback Method
cpg	1279.27	J/mol×K	1033.71	Joback Method
cpg	1312.71	J/mol×K	1070.81	Joback Method
cpg	1348.05	J/mol×K	1107.91	Joback Method
cpg	1385.61	J/mol×K	1145.01	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333549&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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