

larixyl acetate

Inchi: InChI=1S/C24H38O4/c1-9-23(7,28-18(4)26)14-11-19-16(2)15-20(27-17(3)25)21-22(5,6)1
InchiKey: CFEOXVWJRPHLSF-XFWCNITQSA-N
Formula: C24H38O4
SMILES: C=CC(C)(CCC1C(=C)CC(OC(C)=O)C2C(C)(C)CCCC12C)OC(C)=O
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-133.89	kJ/mol	Joback Method
hf	-736.95	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.615		Crippen Method
mcvol	333.580	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2324.00		NIST Webbook
rinpol	2340.00		NIST Webbook
ripol	3185.00		NIST Webbook
ripol	3175.00		NIST Webbook
tb	910.74	K	Joback Method
tc	1131.46	K	Joback Method
tf	575.78	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.35	J/mol×K	910.74	Joback Method
cpg	1178.68	J/mol×K	947.53	Joback Method
cpg	1203.98	J/mol×K	984.31	Joback Method
cpg	1229.49	J/mol×K	1021.10	Joback Method
cpg	1255.44	J/mol×K	1057.89	Joback Method
cpg	1282.07	J/mol×K	1094.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R167218&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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