

(E,Z)-Farnesyl laurate

Inchi:

InChI=1S/C27H48O2/c1-6-7-8-9-10-11-12-13-14-21-27(28)29-23-22-26(5)20-16-19-25(4

InchiKey:

APTQJZOTWYEACL-JBASPHRTSA-N

Formula:

C27H48O2

SMILES:

CCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]:

404.67

Physical Properties

Property code	Value	Unit	Source
gf	157.55	kJ/mol	Joback Method
hf	-523.12	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.870		Crippen Method
mcvol	385.830	ml/mol	McGowan Method
pc	774.61	kPa	Joback Method
ripol	3054.00		NIST Webbook
ripol	3054.00		NIST Webbook
tb	905.57	K	Joback Method
tc	1108.67	K	Joback Method
tf	409.09	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.42	J/mol×K	905.57	Joback Method
cpg	1291.08	J/mol×K	939.42	Joback Method
cpg	1311.67	J/mol×K	973.27	Joback Method
cpg	1331.30	J/mol×K	1007.12	Joback Method
cpg	1350.04	J/mol×K	1040.97	Joback Method
cpg	1368.00	J/mol×K	1074.82	Joback Method
cpg	1385.26	J/mol×K	1108.67	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=R517410&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
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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