

Ligusticumic acid

Inchi:	InChI=1S/C12H14O3/c1-2-3-8-11(13)9-6-4-5-7-10(9)12(14)15/h4-7H,2-3,8H2,1H3,(H,14,
InchiKey:	SWAMOIJQDQZLRX-UHFFFAOYSA-N
Formula:	C12H14O3
SMILES:	CCCCC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]:	206.24
CAS:	550-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-241.72	kJ/mol	Joback Method
hf	-443.34	kJ/mol	Joback Method
hfus	27.77	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.758		Crippen Method
mvol	165.190	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	2004.80		NIST Webbook
rinpol	2004.80		NIST Webbook
tb	705.54	K	Joback Method
tc	908.35	K	Joback Method
tf	424.62	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.96	J/molxK	705.54	Joback Method
cpg	449.14	J/molxK	739.34	Joback Method
cpg	459.60	J/molxK	773.14	Joback Method
cpg	469.38	J/molxK	806.95	Joback Method
cpg	478.50	J/molxK	840.75	Joback Method
cpg	487.00	J/molxK	874.55	Joback Method
cpg	494.91	J/molxK	908.35	Joback Method

dvisc	0.0017112	Paxs	424.62	Joback Method
dvisc	0.0007314	Paxs	471.44	Joback Method
dvisc	0.0003645	Paxs	518.26	Joback Method
dvisc	0.0002038	Paxs	565.08	Joback Method
dvisc	0.0001246	Paxs	611.90	Joback Method
dvisc	0.0000817	Paxs	658.72	Joback Method
dvisc	0.0000567	Paxs	705.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C550378&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mvol:	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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