

Linalyl cinnamate

Inchi:	InChI=1S/C19H24O2/c1-5-19(4,15-9-10-16(2)3)21-18(20)14-13-17-11-7-6-8-12-17/h5-8,
InchiKey:	DPFUEXLIKDHJNB-BUHFOSPRSA-N
Formula:	C19H24O2
SMILES:	<chem>C=CC(C)(CCC=C(C)C)OC(=O)C=Cc1ccccc1</chem>
Mol. weight [g/mol]:	284.39
CAS:	78-37-5

Physical Properties

Property code	Value	Unit	Source
gf	230.16	kJ/mol	Joback Method
hf	-102.43	kJ/mol	Joback Method
hfus	32.19	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.934		Crippen Method
mcvol	249.350	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2082.50		NIST Webbook
rinpol	2082.50		NIST Webbook
rinpol	2131.60		NIST Webbook
tb	738.74	K	Joback Method
tc	956.56	K	Joback Method
tf	379.01	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.13	J/molxK	738.74	Joback Method
cpg	714.41	J/molxK	775.04	Joback Method
cpg	730.55	J/molxK	811.35	Joback Method
cpg	745.66	J/molxK	847.65	Joback Method
cpg	759.83	J/molxK	883.96	Joback Method
cpg	773.17	J/molxK	920.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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