

Cinnamyl linolenate

Inchi:	InChI=1S/C27H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-24-27(28)29-25-20-23-26
InchiKey:	XNIIGWLHWXGQKX-HGXWICJGSA-N
Formula:	C27H38O2
SMILES:	CCC=CCC=CCC=CCCCCCCC(=O)OCC=Cc1cccc1
Mol. weight [g/mol]:	394.59

Physical Properties

Property code	Value	Unit	Source
gf	375.83	kJ/mol	Joback Method
hf	-140.00	kJ/mol	Joback Method
hfus	63.32	kJ/mol	Joback Method
hvap	86.96	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	7.832		Crippen Method
mcvol	357.770	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	3071.60		NIST Webbook
rinpol	3071.60		NIST Webbook
tb	936.77	K	Joback Method
tc	1150.01	K	Joback Method
tf	472.31	K	Joback Method
vc	1.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.07	J/molxK	936.77	Joback Method
cpg	1164.88	J/molxK	972.31	Joback Method
cpg	1182.85	J/molxK	1007.85	Joback Method
cpg	1200.10	J/molxK	1043.39	Joback Method
cpg	1216.74	J/molxK	1078.93	Joback Method
cpg	1232.91	J/molxK	1114.47	Joback Method
cpg	1248.72	J/molxK	1150.01	Joback Method
dvisc	0.0004471	Paxs	472.31	Joback Method

dvisc	0.0001743	Paxs	549.72	Joback Method
dvisc	0.0000857	Paxs	627.13	Joback Method
dvisc	0.0000493	Paxs	704.54	Joback Method
dvisc	0.0000316	Paxs	781.95	Joback Method
dvisc	0.0000220	Paxs	859.36	Joback Method
dvisc	0.0000162	Paxs	936.77	Joback Method

Sources

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=U413751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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<https://www.chemeo.com/cid/86-456-1/Cinnamyl-linolenate.pdf>

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