

cis-3-Hexenylcinnamate

Other names:

Cinnamic acid cis-3-hexenyl ester
2-Propenoic acid, 3-phenyl-, 3(Z)-hexenyl ester
Cinnamic acid, (Z)-3-hexenyl ester
(3Z)-3-Hexenyl 3-phenyl-2-propenoate
(Z)-3-hexenyl cinnamate
(Z)-3-Hexenyl cinnamic ester

Inchi:

InChI=1S/C15H18O2/c1-2-3-4-8-13-17-15(16)12-11-14-9-6-5-7-10-14/h3-7,9-12H,2,8,13

InchiKey:

FKWGVMQNGUQXDN-FECXASIGSA-N

Formula:

C15H18O2

SMILES:

CCC=CCCOC(=O)C=Cc1ccccc1

Mol. weight [g/mol]:

230.30

CAS:

68133-75-5

Physical Properties

Property code	Value	Unit	Source
gf	114.35	kJ/mol	Joback Method
hf	-126.76	kJ/mol	Joback Method
hfus	31.84	kJ/mol	Joback Method
hvap	60.33	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.599		Crippen Method
mcvol	197.290	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1897.00		NIST Webbook
tb	653.89	K	Joback Method
tc	866.88	K	Joback Method
tf	347.23	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.36	J/mol×K	653.89	Joback Method
cpg	519.14	J/mol×K	689.39	Joback Method

cpg	533.92	J/mol×K	724.89	Joback Method
cpg	547.75	J/mol×K	760.38	Joback Method
cpg	560.70	J/mol×K	795.88	Joback Method
cpg	572.83	J/mol×K	831.38	Joback Method
cpg	584.19	J/mol×K	866.88	Joback Method
dvisc	0.0016634	Paxs	347.23	Joback Method
dvisc	0.0007721	Paxs	398.34	Joback Method
dvisc	0.0004267	Paxs	449.45	Joback Method
dvisc	0.0002662	Paxs	500.56	Joback Method
dvisc	0.0001813	Paxs	551.67	Joback Method
dvisc	0.0001317	Paxs	602.78	Joback Method
dvisc	0.0001006	Paxs	653.89	Joback Method

Sources

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=C68133755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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