

Hexanoic acid, 3-phenyl-2-propenyl ester

Other names:	Cinnamyl n-hexanoate Cinnamyl hexanoate
Inchi:	InChI=1S/C15H20O2/c1-2-3-5-12-15(16)17-13-8-11-14-9-6-4-7-10-14/h4,6-11H,2-3,5,12
InchiKey:	BHXVENZBMFLCKE-DHZHZOJOSA-N
Formula:	C15H20O2
SMILES:	CCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	232.32
CAS:	6994-20-3

Physical Properties

Property code	Value	Unit	Source
gf	34.13	kJ/mol	Joback Method
hf	-243.98	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.823		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1805.00		NIST Webbook
ripol	2445.00		NIST Webbook
ripol	2445.00		NIST Webbook
tb	649.73	K	Joback Method
tc	854.73	K	Joback Method
tf	352.31	K	Joback Method
vc	0.771	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.00	J/mol×K	649.73	Joback Method
cpg	597.22	J/mol×K	820.56	Joback Method
cpg	584.55	J/mol×K	786.39	Joback Method
cpg	571.03	J/mol×K	752.23	Joback Method

cpg	556.63	J/molxK	718.06	Joback Method
cpg	541.30	J/molxK	683.90	Joback Method
cpg	609.10	J/molxK	854.73	Joback Method
dvisc	0.0001171	Paxs	649.73	Joback Method
dvisc	0.0001529	Paxs	600.16	Joback Method
dvisc	0.0002096	Paxs	550.59	Joback Method
dvisc	0.0003057	Paxs	501.02	Joback Method
dvisc	0.0004845	Paxs	451.45	Joback Method
dvisc	0.0008601	Paxs	401.88	Joback Method
dvisc	0.0017946	Paxs	352.31	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=C6994203&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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