

2-Propenoic acid, 3-phenyl-, cyclohexyl ester

Other names:	Cinnamic acid, cyclohexyl ester Cyclohexyl cinnamate 2-Butenoic acid,3-phenyl, cyclohexyl ester
Inchi:	InChI=1S/C15H18O2/c16-15(17-14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1,3-4,7-8,11-1
InchiKey:	GCFAUZGWPDYAJN-VAWYXSNFSA-N
Formula:	C15H18O2
SMILES:	O=C(C=Cc1ccccc1)OC1CCCCC1
Mol. weight [g/mol]:	230.30
CAS:	7779-17-1

Physical Properties

Property code	Value	Unit	Source
gf	58.58	kJ/mol	Joback Method
hf	-189.66	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.576		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	669.28	K	Joback Method
tc	909.44	K	Joback Method
tf	359.69	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.14	J/mol×K	669.28	Joback Method
cpg	536.45	J/mol×K	709.31	Joback Method
cpg	554.28	J/mol×K	749.33	Joback Method
cpg	570.70	J/mol×K	789.36	Joback Method
cpg	585.77	J/mol×K	829.39	Joback Method
cpg	599.58	J/mol×K	869.42	Joback Method

cpg	612.19	J/mol×K	909.44	Joback Method
dvisc	0.0021688	Pa×s	359.69	Joback Method
dvisc	0.0009981	Pa×s	411.29	Joback Method
dvisc	0.0005461	Pa×s	462.89	Joback Method
dvisc	0.0003372	Pa×s	514.49	Joback Method
dvisc	0.0002274	Pa×s	566.08	Joback Method
dvisc	0.0001637	Pa×s	617.68	Joback Method
dvisc	0.0001240	Pa×s	669.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7779171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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