Benzenepropanoic acid, 3-phenyl-2-propenyl ester

Other names: Cinnamyl-«beta»-phenylpropionate
Cinnamyl 3-phenylpropanoate
Inchi: InChI=1S/C18H18O2/c19-18(14-13-17-10-5-2-6-11-17)20-15-7-12-16-8-3-1-4-9-16/h1-12
InchiKey: SYPODLJMXGVBQI-KPKJPENVSA-N
Formula: C18H18O2
SMILES: O=C(CCc1ccccc1)OCC=Cc1ccccc1
Mol. weight [g/mol]: 266.33
CAS: 28048-98-8

Physical Properties

Property code	Value	Unit	Source
gf	171.80	kJ/mol	Joback Method
hf	-69.37	kJ/mol	Joback Method
hfus	33.45	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.876		Crippen Method
mcvol	220.100	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2250.20		NIST Webbook
rinpol	2250.20		NIST Webbook
tb	745.05	K	Joback Method
tc	978.05	K	Joback Method
tf	412.54	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.39	J/mol×K	745.05	Joback Method
cpg	618.52	J/mol×K	783.88	Joback Method
cpg	633.41	J/mol×K	822.72	Joback Method
cpg	647.13	J/mol×K	861.55	Joback Method
cpg	659.78	J/mol×K	900.38	Joback Method

cpg	671.42	J/mol×K	939.22	Joback Method
cpg	682.16	J/mol×K	978.05	Joback Method
dvisc	0.0011452	Pa×s	412.54	Joback Method
dvisc	0.0005723	Pa×s	467.96	Joback Method
dvisc	0.0003312	Pa×s	523.38	Joback Method
dvisc	0.0002129	Pa×s	578.80	Joback Method
dvisc	0.0001478	Pa×s	634.21	Joback Method
dvisc	0.0001088	Pa×s	689.63	Joback Method
dvisc	0.0000838	Pa×s	745.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28048988&Units=SI

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