Cinnamyl cinnamate

Other names:	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propenyl ester
	Cinnamic acid, cinnamyl ester
	Cinnamyl alcohol, cinnamate
	Phenylallyl cinnamate
	Styracin
	3-Phenyl-2-propen-1-yl cinnamate
	Cinnamylester kyseliny skoricove
	3-Phenyl-2-propen-1-yl 3-phenyl propenoate
	3-Phenyl allyl cinnamate
	Cinnamyl «beta»-phenylacrylate
	2-Propenoic acid, 3-phenyl-, 3-phenyl-2-propen-1-yl ester
	NSC 46161
Inchi:	InChI=1S/C18H16O2/c19-18(14-13-17-10-5-2-6-11-17)20-15-7-12-16-8-3-1-4-9-16/h1-14
InchiKey:	NQBWNECTZUOWID-UHFFFAOYSA-N
Formula:	C18H16O2
SMILES:	O=C(C=Cc1ccccc1)OCC=Cc1ccccc1
Mol. weight [g/mol]:	264.32
CAS:	122-69-0

Physical Properties

Property code	Value	Unit	Source
gf	252.02	kJ/mol	Joback Method
hf	47.85	kJ/mol	Joback Method
hfus	33.65	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.956		Crippen Method
mcvol	215.800	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2447.00		NIST Webbook
tb	749.21	K	Joback Method
tc	991.03	K	Joback Method
tf	407.46	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.88	J/mol×K	749.21	Joback Method
cpg	644.51	J/mol×K	950.72	Joback Method
cpg	633.21	J/mol×K	910.42	Joback Method
cpg	621.01	J/mol×K	870.12	Joback Method
cpg	607.80	J/mol×K	829.82	Joback Method
cpg	593.46	J/mol×K	789.51	Joback Method
cpg	655.03	J/mol×K	991.03	Joback Method
dvisc	0.0000726	Pa×s	749.21	Joback Method
dvisc	0.0000945	Pa×s	692.25	Joback Method
dvisc	0.0001288	Pa×s	635.29	Joback Method
dvisc	0.0001867	Pa×s	578.34	Joback Method
dvisc	0.0002933	Pa×s	521.38	Joback Method
dvisc	0.0005150	Pa×s	464.42	Joback Method
dvisc	0.0010583	Pa×s	407.46	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=C122690&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

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