BENZYL CINNAMATE

Other names:	2-Propenoic acid, 3-phenyl-, phenylmethyl ester
	Benzyl «gamma»-phenylacrylate
	Benzyl alcohol cinnamic ester
	Benzyl alcohol, cinnamate
	Cinnamein
	Cinnamic acid, benzyl ester
	Benzylester kyseliny skoricove
	3-Phenyl-2-propenoic acid phenylmethyl ester
	Benzyl 3-phenylpropenoate
	Benzyl 3-phenyl-2-propenoate
	NSC 11780
Inchi:	InChI=1S/C16H14O2/c17-16(12-11-14-7-3-1-4-8-14)18-13-15-9-5-2-6-10-15/h1-12H,13H
InchiKey:	NGHOLYJTSCBCGC-VAWYXSNFSA-N
Formula:	C16H14O2
SMILES:	O=C(/C=C/c1ccccc1)OCc1ccccc1
Mol. weight [g/mol]:	238.29

Physical Properties

Property code	Value	Unit	Source
hf	-79.97	kJ/mol	Cheméo Relay (1.0)
hfus	28.27	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-4.56		Cheméo Relay (1.0)
logp	3.443		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
rinpol	2138.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2096.00		NIST Webbook
ripol	2769.00		NIST Webbook
ripol	2769.00		NIST Webbook

tb	617.78	K	Cheméo Relay (1.0)
tf	333.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.58	J/mol×K	901.28	Joback Method
cpg	571.63	J/mol×K	941.67	Joback Method
cpg	511.23	J/mol×K	739.69	Joback Method
cpg	525.51	J/mol×K	780.08	Joback Method
cpg	538.61	J/mol×K	820.48	Joback Method
cpg	550.60	J/mol×K	860.88	Joback Method
cpg	495.69	J/mol×K	699.29	Joback Method
dvisc	0.0003999	Pa×s	493.10	Joback Method
dvisc	0.0006777	Pa×s	441.55	Joback Method
dvisc	0.0013204	Pa×s	390.00	Joback Method
dvisc	0.0002607	Pa×s	544.64	Joback Method
dvisc	0.0001830	Pa×s	596.19	Joback Method
dvisc	0.0001359	Pa×s	647.74	Joback Method
dvisc	0.0001055	Pa×s	699.29	Joback Method
hvapt	89.40	kJ/mol	534.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103413&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point