

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=Cc1ccccc1)OCc1ccccc1

Mol. weight [g/mol]:

238.28

CAS:

103-41-3

Physical Properties

Property code	Value	Unit	Source
gf	154.96	kJ/mol	Joback Method
hf	-28.09	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.443		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2135.00		NIST Webbook

ripol	2769.00		NIST Webbook
ripol	2769.00		NIST Webbook
tb	699.29	K	Joback Method
tc	941.67	K	Joback Method
tf	390.00	K	Joback Method
vc	0.720	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.69	J/mol×K	699.29	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	561.58	J/mol×K	901.28	Joback Method
cpg	571.63	J/mol×K	941.67	Joback Method
dvisc	0.0013204	Paxs	390.00	Joback Method
dvisc	0.0006777	Paxs	441.55	Joback Method
dvisc	0.0003999	Paxs	493.10	Joback Method
dvisc	0.0002607	Paxs	544.64	Joback Method
dvisc	0.0001830	Paxs	596.19	Joback Method
dvisc	0.0001359	Paxs	647.74	Joback Method
dvisc	0.0001055	Paxs	699.29	Joback Method
hvapt	89.40	kJ/mol	534.50	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C103413&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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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