

Allyl cinnamate

Other names:	2-Propenoic acid, 3-phenyl-, 2-propenyl ester Cinnamic acid, allyl ester Allyl 3-phenylacrylate Propenyl cinnamate Vinyl carbinyl cinnamate Allylester kyseliny skoricove Allyl 3-phenyl-2-propenoate 2-Propenoic acid, 3-phenyl-, 2-propen-1-yl ester NSC 20972
Inchi:	InChI=1S/C12H12O2/c1-2-10-14-12(13)9-8-11-6-4-3-5-7-11/h2-9H,1,10H2/b9-8+
InchiKey:	KCMITHMNVLRGJU-CMDGGOBGSA-N
Formula:	C12H12O2
SMILES:	<chem>C=CCOC(=O)C=Cc1ccccc1</chem>
Mol. weight [g/mol]:	188.22
CAS:	1866-31-5

Physical Properties

Property code	Value	Unit	Source
gf	96.71	kJ/mol	Joback Method
hf	-56.63	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	53.03	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.429		Crippen Method
mcvol	155.020	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1537.00		NIST Webbook
rinpol	1524.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2258.00		NIST Webbook
tb	577.77	K	Joback Method
tc	797.26	K	Joback Method
tf	316.74	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.11	J/molxK	577.77	Joback Method
cpg	368.11	J/molxK	614.35	Joback Method
cpg	381.18	J/molxK	650.93	Joback Method
cpg	393.37	J/molxK	687.52	Joback Method
cpg	404.73	J/molxK	724.10	Joback Method
cpg	415.30	J/molxK	760.68	Joback Method
cpg	425.13	J/molxK	797.26	Joback Method
dvisc	0.0019746	Paxs	316.74	Joback Method
dvisc	0.0010120	Paxs	360.25	Joback Method
dvisc	0.0005990	Paxs	403.75	Joback Method
dvisc	0.0003927	Paxs	447.25	Joback Method
dvisc	0.0002774	Paxs	490.76	Joback Method
dvisc	0.0002074	Paxs	534.26	Joback Method
dvisc	0.0001620	Paxs	577.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1866315&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
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

Latest version available from:

<https://www.cheméo.com/cid/85-612-8/Allyl-cinnamate.pdf>

Generated by Cheméo on 2024-09-08 06:13:57.190261374 +0000 UTC m=+356899.827230621.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.