Benzeneacetic acid, 3-phenyl-2-propenyl ester

Other names: Benzeneacetic acid, 3-phenyl-2-propyl ester
cinnamyl phenylacetate
Inchi: InChI=1S/C17H16O2/c18-17(14-16-10-5-2-6-11-16)19-13-7-12-15-8-3-1-4-9-15/h1-12H,1
InchiKey: SFXQCOMMEMBETJ-KPKJPENVSA-N
Formula: C17H16O2
SMILES: O=C(Cc1ccccc1)OCC=Cc1ccccc1
Mol. weight [g/mol]: 252.31
CAS: 7492-65-1

Physical Properties

Property code	Value	Unit	Source
gf	163.38	kJ/mol	Joback Method
hf	-48.73	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.486		Crippen Method
mcvol	206.010	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1820.00		NIST Webbook
tb	722.17	K	Joback Method
tc	959.64	K	Joback Method
tf	401.27	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.46	J/mol×K	722.17	Joback Method
cpg	564.34	J/mol×K	761.75	Joback Method
cpg	578.95	J/mol×K	801.33	Joback Method
cpg	592.39	J/mol×K	840.90	Joback Method
cpg	604.74	J/mol×K	880.48	Joback Method
cpg	616.08	J/mol×K	920.06	Joback Method

cpg	626.50	J/mol×K	959.64	Joback Method
dvisc	0.0012341	Pa×s	401.27	Joback Method
dvisc	0.0006248	Pa×s	454.75	Joback Method
dvisc	0.0003650	Pa×s	508.24	Joback Method
dvisc	0.0002362	Pa×s	561.72	Joback Method
dvisc	0.0001649	Pa×s	615.20	Joback Method
dvisc	0.0001219	Pa×s	668.69	Joback Method
dvisc	0.0000943	Pa×s	722.17	Joback Method

Sources

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=C7492651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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