

Benzeneacetic acid, 2-propenyl ester

Other names:	Acetic acid, phenyl-, allyl ester Allyl phenylacetate Phenylacetic acid allyl ester 2-Propenyl phenylacetate
Inchi:	InChI=1S/C11H12O2/c1-2-8-13-11(12)9-10-6-4-3-5-7-10/h2-7H,1,8-9H2
InchiKey:	ZCDYAMJXVAUTIM-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	<chem>C=CCOC(=O)Cc1ccccc1</chem>
Mol. weight [g/mol]:	176.21
CAS:	1797-74-6

Physical Properties

Property code	Value	Unit	Source
gf	8.07	kJ/mol	Joback Method
hf	-153.21	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.958		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1328.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2175.00		NIST Webbook
tb	550.73	K	Joback Method
tc	764.42	K	Joback Method
tf	310.55	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.91	J/mol×K	550.73	Joback Method
cpg	340.70	J/mol×K	586.34	Joback Method
cpg	353.66	J/mol×K	621.96	Joback Method
cpg	365.82	J/mol×K	657.57	Joback Method
cpg	377.21	J/mol×K	693.19	Joback Method
cpg	387.86	J/mol×K	728.80	Joback Method
cpg	397.79	J/mol×K	764.42	Joback Method
dvisc	0.0021881	Paxs	310.55	Joback Method
dvisc	0.0011786	Paxs	350.58	Joback Method
dvisc	0.0007207	Paxs	390.61	Joback Method
dvisc	0.0004829	Paxs	430.64	Joback Method
dvisc	0.0003463	Paxs	470.67	Joback Method
dvisc	0.0002617	Paxs	510.70	Joback Method
dvisc	0.0002060	Paxs	550.73	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=C1797746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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