Allyl phenoxyacetate

Other names:	Acetic acid, phenoxy-, 2-propenyl ester
	Acetate p.a.
	Acetic acid, phenoxy-, allyl ester
Inchi:	InChI=1S/C11H12O3/c1-2-8-13-11(12)9-14-10-6-4-3-5-7-10/h2-7H,1,8-9H2
InchiKey:	VUFZVGQUAVDKMC-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	C=CCOC(=O)COc1ccccc1
Mol. weight [g/mol]:	192.21
CAS:	7493-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-96.93	kJ/mol	Joback Method
hf	-285.43	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.795		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	573.15	K	Joback Method
tc	784.49	K	Joback Method
tf	332.78	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.11	J/mol×K	573.15	Joback Method
cpg	364.61	J/mol×K	608.37	Joback Method

cpg	377.34	J/mol×K	643.60	Joback Method
cpg	389.31	J/mol×K	678.82	Joback Method
cpg	400.55	J/mol×K	714.04	Joback Method
cpg	411.06	J/mol×K	749.26	Joback Method
cpg	420.85	J/mol×K	784.49	Joback Method
dvisc	0.0016305	Pa×s	332.78	Joback Method
dvisc	0.0009104	Pa×s	372.84	Joback Method
dvisc	0.0005692	Pa×s	412.90	Joback Method
dvisc	0.0003867	Pa×s	452.96	Joback Method
dvisc	0.0002797	Pa×s	493.03	Joback Method
dvisc	0.0002125	Pa×s	533.09	Joback Method
dvisc	0.0001677	Pa×s	573.15	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=C7493745&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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