Allylphenoxy acetate

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

Physical Properties

Property code	Value	Unit	Source
hfus	20.98	kJ/mol	Joback Method
log10ws	-2.37		Cheméo Relay (1.0)
logp	1.795		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
rinpol	1452.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	548.13	K	Cheméo Relay (1.0)
tf	280.40	K	Cheméo Relay (1.0)

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	452.97	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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7493745&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point