Allyl methyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, allyl methyl ester
Inchi: InChI=1S/C12H12O4/c1-3-8-16-12(14)10-7-5-4-6-9(10)11(13)15-2/h3-7H,1,8H2,2H3
InchiKey: CGSRKECNVRWYOK-UHFFFAOYSA-N
Formula: C12H12O4
SMILES: C=CCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 220.22

Physical Properties

Property code	Value	Unit	Source
gf	-227.06	kJ/mol	Joback Method
hf	-430.12	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.816		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	654.88	K	Joback Method
tc	870.69	K	Joback Method
tf	406.50	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.18	J/mol×K	654.88	Joback Method
cpg	426.87	J/mol×K	690.85	Joback Method
cpg	438.76	J/mol×K	726.82	Joback Method
cpg	449.84	J/mol×K	762.79	Joback Method
cpg	460.14	J/mol×K	798.75	Joback Method
cpg	469.64	J/mol×K	834.72	Joback Method
cpg	478.37	J/mol×K	870.69	Joback Method

dvisc	0.0011013	Pa×s	406.50	Joback Method
dvisc	0.0006841	Pa×s	447.90	Joback Method
dvisc	0.0004606	Pa×s	489.29	Joback Method
dvisc	0.0003299	Pa×s	530.69	Joback Method
dvisc	0.0002480	Pa×s	572.09	Joback Method
dvisc	0.0001937	Pa×s	613.48	Joback Method
dvisc	0.0001561	Pa×s	654.88	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=U373891&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