Phthalic acid, allyl ethyl ester

Other names: Ethylallylphthalate
Inchi: InChI=1S/C13H14O4/c1-3-9-17-13(15)11-8-6-5-7-10(11)12(14)16-4-2/h3,5-8H,1,4,9H2,2
InchiKey: UPBGNLFFUITRLL-UHFFFAOYSA-N
Formula: C13H14O4
SMILES: C=CCOC(=O)c1ccccc1C(=O)OCC
Mol. weight [g/mol]: 234.25
CAS: 33672-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-218.64	kJ/mol	Joback Method
hf	-450.76	kJ/mol	Joback Method
hfus	27.37	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.206		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	1776.00		NIST Webbook
tb	677.76	K	Joback Method
tc	890.16	K	Joback Method
tf	417.77	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.54	J/mol×K	677.76	Joback Method
cpg	477.83	J/mol×K	713.16	Joback Method
cpg	490.27	J/mol×K	748.56	Joback Method
cpg	501.86	J/mol×K	783.96	Joback Method
cpg	512.63	J/mol×K	819.36	Joback Method
cpg	522.58	J/mol×K	854.76	Joback Method
cpg	531.71	J/mol×K	890.16	Joback Method

dvisc	0.0010467	Pa×s	417.77	Joback Method
dvisc	0.0006399	Pa×s	461.10	Joback Method
dvisc	0.0004256	Pa×s	504.43	Joback Method
dvisc	0.0003020	Pa×s	547.76	Joback Method
dvisc	0.0002253	Pa×s	591.10	Joback Method
dvisc	0.0001750	Pa×s	634.43	Joback Method
dvisc	0.0001404	Pa×s	677.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C33672945&Units=SI

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