

Acetic acid, (4-chlorophenoxy)-, pentyl ester

Inchi:	InChI=1S/C13H17ClO3/c1-2-3-4-9-16-13(15)10-17-12-7-5-11(14)6-8-12/h5-8H,2-4,9-10H
InchiKey:	JTQBAUWCCUBO AQ-UHFFFAOYSA-N
Formula:	C13H17ClO3
SMILES:	CCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	256.73

Physical Properties

Property code	Value	Unit	Source
gf	-189.49	kJ/mol	Joback Method
hf	-479.35	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	63.42	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.452		Crippen Method
mvol	195.820	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	2273.00		NIST Webbook
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tb	664.64	K	Joback Method
tc	870.26	K	Joback Method
tf	399.52	K	Joback Method
vc	0.747	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.37	J/molxK	664.64	Joback Method
cpg	511.71	J/molxK	698.91	Joback Method
cpg	525.21	J/molxK	733.18	Joback Method
cpg	537.89	J/molxK	767.45	Joback Method
cpg	549.74	J/molxK	801.72	Joback Method
cpg	560.79	J/molxK	835.99	Joback Method
cpg	571.04	J/molxK	870.26	Joback Method
dvisc	0.0010749	Paxs	399.52	Joback Method

dvisc	0.0006245	Paxs	443.71	Joback Method
dvisc	0.0004004	Paxs	487.89	Joback Method
dvisc	0.0002763	Paxs	532.08	Joback Method
dvisc	0.0002019	Paxs	576.27	Joback Method
dvisc	0.0001542	Paxs	620.45	Joback Method
dvisc	0.0001221	Paxs	664.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415097&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

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