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

Inchi: InChI=1S/C19H29ClO3/c1-2-3-4-5-6-7-8-9-10-15-22-19(21)16-23-18-13-11-17(20)12-14-
InchiKey: LBIRRDZXSMKWGD-UHFFFAOYSA-N
Formula: C19H29ClO3
SMILES: CCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 340.88

Physical Properties

Property code	Value	Unit	Source
gf	-138.97	kJ/mol	Joback Method
hf	-603.19	kJ/mol	Joback Method
hfus	46.79	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.793		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	3005.00		NIST Webbook
tb	801.92	K	Joback Method
tc	998.51	K	Joback Method
tf	467.14	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.37	J/mol×K	801.92	Joback Method
cpg	844.82	J/mol×K	834.68	Joback Method
cpg	860.22	J/mol×K	867.45	Joback Method
cpg	874.60	J/mol×K	900.21	Joback Method
cpg	887.97	J/mol×K	932.98	Joback Method
cpg	900.36	J/mol×K	965.74	Joback Method
cpg	911.78	J/mol×K	998.51	Joback Method
dvisc	0.0006583	Pa×s	467.14	Joback Method
dvisc	0.0003518	Pa×s	522.94	Joback Method

dvisc	0.0002122	Pa×s	578.73	Joback Method
dvisc	0.0001398	Pa×s	634.53	Joback Method
dvisc	0.0000986	Pa×s	690.33	Joback Method
dvisc	0.0000732	Pa×s	746.12	Joback Method
dvisc	0.0000567	Pa×s	801.92	Joback Method

Sources

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=U415104&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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