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

Inchi: InChI=1S/C23H37ClO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-26-23(25)20-27-22-17-15-
InchiKey: GNJJCFNQBVHWNR-UHFFFAOYSA-N
Formula: C23H37ClO3
SMILES: CCCCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 396.99

Physical Properties

Property code	Value	Unit	Source
gf	-105.29	kJ/mol	Joback Method
hf	-685.75	kJ/mol	Joback Method
hfus	57.15	kJ/mol	Joback Method
hvap	85.68	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.353		Crippen Method
mcvol	336.720	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	893.44	K	Joback Method
tc	1096.12	K	Joback Method
tf	512.22	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.83	J/mol×K	893.44	Joback Method
cpg	1085.26	J/mol×K	927.22	Joback Method
cpg	1101.45	J/mol×K	961.00	Joback Method
cpg	1116.44	J/mol×K	994.78	Joback Method
cpg	1130.25	J/mol×K	1028.56	Joback Method
cpg	1142.92	J/mol×K	1062.34	Joback Method
cpg	1154.50	J/mol×K	1096.12	Joback Method
dvisc	0.0004303	Pa×s	512.22	Joback Method

dvisc	0.0002197	Pa×s	575.76	Joback Method
dvisc	0.0001282	Pa×s	639.29	Joback Method
dvisc	0.0000825	Pa×s	702.83	Joback Method
dvisc	0.0000571	Pa×s	766.37	Joback Method
dvisc	0.0000418	Pa×s	829.90	Joback Method
dvisc	0.0000320	Pa×s	893.44	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=U415108&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