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

Inchi: InChI=1S/C22H35ClO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-25-22(24)19-26-21-16-14-20(

InchiKey: DQJWGWASPUUPQY-UHFFFAOYSA-N

Formula: C22H35ClO3

SMILES: CCCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1

Mol. weight [g/mol]: 382.96

Physical Properties

Property code	Value	Unit	Source
gf	-113.71	kJ/mol	Joback Method
hf	-665.11	kJ/mol	Joback Method
hfus	54.56	kJ/mol	Joback Method
hvap	83.45	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.963		Crippen Method
mcvol	322.630	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	870.56	K	Joback Method
tc	1070.58	K	Joback Method
tf	500.95	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.88	J/mol×K	870.56	Joback Method
cpg	1024.06	J/mol×K	903.90	Joback Method
cpg	1040.05	J/mol×K	937.23	Joback Method
cpg	1054.89	J/mol×K	970.57	Joback Method
cpg	1068.60	J/mol×K	1003.90	Joback Method
cpg	1081.23	J/mol×K	1037.24	Joback Method
cpg	1092.80	J/mol×K	1070.58	Joback Method
dvisc	0.0004814	Pa×s	500.95	Joback Method

dvisc	0.0002484	Pa×s	562.55	Joback Method
dvisc	0.0001461	Pa×s	624.15	Joback Method
dvisc	0.0000945	Pa×s	685.75	Joback Method
dvisc	0.0000657	Pa×s	747.36	Joback Method
dvisc	0.0000483	Pa×s	808.96	Joback Method
dvisc	0.0000370	Pa×s	870.56	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=U415107&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