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

Inchi: InChI=1S/C26H43ClO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-29-26(28)23-30-
InchiKey: MUMWTAAGZDVYGP-UHFFFAOYSA-N
Formula: C26H43ClO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 439.07

Physical Properties

Property code	Value	Unit	Source
gf	-80.03	kJ/mol	Joback Method
hf	-747.67	kJ/mol	Joback Method
hfus	64.92	kJ/mol	Joback Method
hvap	92.36	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	8.523		Crippen Method
mcvol	378.990	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	962.08	K	Joback Method
tc	1178.19	K	Joback Method
tf	546.03	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.15	J/mol×K	962.08	Joback Method
cpg	1272.49	J/mol×K	998.10	Joback Method
cpg	1289.36	J/mol×K	1034.12	Joback Method
cpg	1304.81	J/mol×K	1070.14	Joback Method
cpg	1318.89	J/mol×K	1106.16	Joback Method
cpg	1331.65	J/mol×K	1142.17	Joback Method
cpg	1343.15	J/mol×K	1178.19	Joback Method
dvisc	0.0003014	Pa×s	546.03	Joback Method

dvisc	0.0001493	Pa×s	615.37	Joback Method
dvisc	0.0000853	Pa×s	684.71	Joback Method
dvisc	0.0000540	Pa×s	754.05	Joback Method
dvisc	0.0000369	Pa×s	823.40	Joback Method
dvisc	0.0000268	Pa×s	892.74	Joback Method
dvisc	0.0000204	Pa×s	962.08	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=U415111&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