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

Inchi: InChI=1S/C25H41ClO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-28-25(27)22-29-24-
InchiKey: GYFITDNLYCLDPF-UHFFFAOYSA-N
Formula: C25H41ClO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 425.04

Physical Properties

Property code	Value	Unit	Source
gf	-88.45	kJ/mol	Joback Method
hf	-727.03	kJ/mol	Joback Method
hfus	62.33	kJ/mol	Joback Method
hvap	90.13	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.133		Crippen Method
mcvol	364.900	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	939.20	K	Joback Method
tc	1149.86	K	Joback Method
tf	534.76	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.52	J/mol×K	939.20	Joback Method
cpg	1209.53	J/mol×K	974.31	Joback Method
cpg	1226.15	J/mol×K	1009.42	Joback Method
cpg	1241.44	J/mol×K	1044.53	Joback Method
cpg	1255.43	J/mol×K	1079.64	Joback Method
cpg	1268.18	J/mol×K	1114.75	Joback Method
cpg	1279.72	J/mol×K	1149.86	Joback Method
dvisc	0.0003404	Pa×s	534.76	Joback Method

dvisc	0.0001703	Pa×s	602.17	Joback Method
dvisc	0.0000980	Pa×s	669.57	Joback Method
dvisc	0.0000623	Pa×s	736.98	Joback Method
dvisc	0.0000428	Pa×s	804.39	Joback Method
dvisc	0.0000311	Pa×s	871.79	Joback Method
dvisc	0.0000237	Pa×s	939.20	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=U415110&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