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

Inchi: InChI=1S/C21H33ClO3/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)18-25-20-15-13-19(22)
InchiKey: UVORFUCIVQTNPB-UHFFFAOYSA-N
Formula: C21H33ClO3
SMILES: CCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 368.94

Physical Properties

Property code	Value	Unit	Source
gf	-122.13	kJ/mol	Joback Method
hf	-644.47	kJ/mol	Joback Method
hfus	51.97	kJ/mol	Joback Method
hvap	81.23	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.573		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
tb	847.68	K	Joback Method
tc	1045.83	K	Joback Method
tf	489.68	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.61	J/mol×K	847.68	Joback Method
cpg	963.54	J/mol×K	880.70	Joback Method
cpg	979.34	J/mol×K	913.73	Joback Method
cpg	994.03	J/mol×K	946.75	Joback Method
cpg	1007.65	J/mol×K	979.78	Joback Method
cpg	1020.21	J/mol×K	1012.80	Joback Method
cpg	1031.75	J/mol×K	1045.83	Joback Method
dvisc	0.0005365	Pa×s	489.68	Joback Method

dvisc	0.0002800	Pa×s	549.35	Joback Method
dvisc	0.0001660	Pa×s	609.01	Joback Method
dvisc	0.0001080	Pa×s	668.68	Joback Method
dvisc	0.0000754	Pa×s	728.35	Joback Method
dvisc	0.0000556	Pa×s	788.01	Joback Method
dvisc	0.0000428	Pa×s	847.68	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=U415106&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