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

Inchi: InChI=1S/C20H31ClO3/c1-2-3-4-5-6-7-8-9-10-11-16-23-20(22)17-24-19-14-12-18(21)13-
InchiKey: AADXTAYPDHMYDB-UHFFFAOYSA-N
Formula: C20H31ClO3
SMILES: CCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 354.91

Physical Properties

Property code	Value	Unit	Source
gf	-130.55	kJ/mol	Joback Method
hf	-623.83	kJ/mol	Joback Method
hfus	49.38	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.183		Crippen Method
mcvol	294.450	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		NIST Webbook
tb	824.80	K	Joback Method
tc	1021.83	K	Joback Method
tf	478.41	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.09	J/mol×K	824.80	Joback Method
cpg	903.78	J/mol×K	857.64	Joback Method
cpg	919.38	J/mol×K	890.48	Joback Method
cpg	933.92	J/mol×K	923.31	Joback Method
cpg	947.42	J/mol×K	956.15	Joback Method
cpg	959.91	J/mol×K	988.99	Joback Method
cpg	971.40	J/mol×K	1021.83	Joback Method
dvisc	0.0005955	Pa×s	478.41	Joback Method

dvisc	0.0003144	Pa×s	536.14	Joback Method
dvisc	0.0001880	Pa×s	593.87	Joback Method
dvisc	0.0001231	Pa×s	651.61	Joback Method
dvisc	0.0000864	Pa×s	709.34	Joback Method
dvisc	0.0000639	Pa×s	767.07	Joback Method
dvisc	0.0000493	Pa×s	824.80	Joback Method

Sources

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=U415105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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