Pimelic acid, 3-chlorophenyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C19H27ClO4/c1-14(2)12-15(3)23-18(21)10-5-4-6-11-19(22)24-17-9-7-8-16(20)

InchiKey: CZQLPJWCLRPJIJ-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-272.77	kJ/mol	Joback Method
hf	-726.33	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.174		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook
tb	854.91	K	Joback Method
tc	1063.12	K	Joback Method
tf	487.07	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.35	J/mol×K	854.91	Joback Method
cpg	910.86	J/mol×K	1028.42	Joback Method
cpg	900.40	J/mol×K	993.72	Joback Method
cpg	888.84	J/mol×K	959.02	Joback Method
cpg	876.17	J/mol×K	924.31	Joback Method
cpg	862.34	J/mol×K	889.61	Joback Method
cpg	920.25	J/mol×K	1063.12	Joback Method
dvisc	0.0000458	Pa×s	854.91	Joback Method

dvisc	0.0000604	Pa×s	793.60	Joback Method
dvisc	0.0000834	Pa×s	732.30	Joback Method
dvisc	0.0001223	Pa×s	670.99	Joback Method
dvisc	0.0001936	Pa×s	609.68	Joback Method
dvisc	0.0003396	Pa×s	548.38	Joback Method
dvisc	0.0006863	Pa×s	487.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416671&Units=SI
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

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