Pimelic acid, 3-chlorophenyl pentyl ester

Inchi: InChI=1S/C18H25ClO4/c1-2-3-7-13-22-17(20)11-5-4-6-12-18(21)23-16-10-8-9-15(19)14-
InchiKey: FQOPPUXDFFWXOW-UHFFFAOYSA-N
Formula: C18H25ClO4
SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-276.31	kJ/mol	Joback Method
hf	-695.13	kJ/mol	Joback Method
hfus	45.80	kJ/mol	Joback Method
hvap	81.30	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.929		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook
tb	832.91	K	Joback Method
tc	1037.04	K	Joback Method
tf	505.80	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.39	J/mol×K	832.91	Joback Method
cpg	850.59	J/mol×K	1003.02	Joback Method
cpg	840.20	J/mol×K	968.99	Joback Method
cpg	828.80	J/mol×K	934.97	Joback Method
cpg	816.38	J/mol×K	900.95	Joback Method
cpg	802.92	J/mol×K	866.93	Joback Method
cpg	860.00	J/mol×K	1037.04	Joback Method
dvisc	0.0000629	Pa×s	832.91	Joback Method

dvisc	0.0000802	Pa×s	778.39	Joback Method
dvisc	0.0001061	Pa×s	723.87	Joback Method
dvisc	0.0001470	Pa×s	669.36	Joback Method
dvisc	0.0002157	Pa×s	614.84	Joback Method
dvisc	0.0003411	Pa×s	560.32	Joback Method
dvisc	0.0005954	Pa×s	505.80	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=U416672&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