Pimelic acid, 4-chlorophenyl hexyl ester

Inchi: InChI=1S/C19H27ClO4/c1-2-3-4-8-15-23-18(21)9-6-5-7-10-19(22)24-17-13-11-16(20)12-
InchiKey: BVSBZHVJESNBHV-UHFFFAOYSA-N
Formula: C19H27ClO4
SMILES: CCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-267.89	kJ/mol	Joback Method
hf	-715.77	kJ/mol	Joback Method
hfus	48.39	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.319		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	855.79	K	Joback Method
tc	1060.17	K	Joback Method
tf	517.07	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.29	J/mol×K	855.79	Joback Method
cpg	861.04	J/mol×K	889.85	Joback Method
cpg	874.69	J/mol×K	923.92	Joback Method
cpg	887.26	J/mol×K	957.98	Joback Method
cpg	898.76	J/mol×K	992.04	Joback Method
cpg	909.23	J/mol×K	1026.10	Joback Method
cpg	918.69	J/mol×K	1060.17	Joback Method
dvisc	0.0005380	Pa×s	517.07	Joback Method

dvisc	0.0003045	Pa×s	573.52	Joback Method
dvisc	0.0001909	Pa×s	629.98	Joback Method
dvisc	0.0001292	Pa×s	686.43	Joback Method
dvisc	0.0000928	Pa×s	742.88	Joback Method
dvisc	0.0000698	Pa×s	799.34	Joback Method
dvisc	0.0000546	Pa×s	855.79	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=U393832&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