Pimelic acid, 4-chlorophenyl undecyl ester

Inchi: InChI=1S/C24H37ClO4/c1-2-3-4-5-6-7-8-9-13-20-28-23(26)14-11-10-12-15-24(27)29-22-
InchiKey: BXFYFHYNGQGJQG-UHFFFAOYSA-N
Formula: C24H37ClO4
SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 425.00

Physical Properties

Property code	Value	Unit	Source
gf	-225.79	kJ/mol	Joback Method
hf	-818.97	kJ/mol	Joback Method
hfus	61.34	kJ/mol	Joback Method
hvap	94.65	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.270		Crippen Method
mcvol	352.380	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	3097.00		NIST Webbook
rinpol	3097.00		NIST Webbook
tb	970.19	K	Joback Method
tc	1187.80	K	Joback Method
tf	573.42	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.11	J/mol×K	970.19	Joback Method
cpg	1161.98	J/mol×K	1006.46	Joback Method
cpg	1176.44	J/mol×K	1042.73	Joback Method
cpg	1189.54	J/mol×K	1079.00	Joback Method
cpg	1201.32	J/mol×K	1115.26	Joback Method
cpg	1211.83	J/mol×K	1151.53	Joback Method
cpg	1221.10	J/mol×K	1187.80	Joback Method
dvisc	0.0003068	Pa×s	573.42	Joback Method

dvisc	0.0001644	Pa×s	639.55	Joback Method
dvisc	0.0000990	Pa×s	705.68	Joback Method
dvisc	0.0000650	Pa×s	771.81	Joback Method
dvisc	0.0000457	Pa×s	837.93	Joback Method
dvisc	0.0000338	Pa×s	904.06	Joback Method
dvisc	0.0000260	Pa×s	970.19	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=U393837&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