Pimelic acid, 4-chlorophenyl dodecyl ester

Inchi: InChI=1S/C25H39ClO4/c1-2-3-4-5-6-7-8-9-10-14-21-29-24(27)15-12-11-13-16-25(28)30-
InchiKey: QALMZZGZMCIJTF-UHFFFAOYSA-N
Formula: C25H39ClO4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 439.03

Physical Properties

Property code	Value	Unit	Source
gf	-217.37	kJ/mol	Joback Method
hf	-839.61	kJ/mol	Joback Method
hfus	63.93	kJ/mol	Joback Method
hvap	96.88	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	7.660		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	993.07	K	Joback Method
tc	1216.15	K	Joback Method
tf	584.69	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.72	J/mol×K	993.07	Joback Method
cpg	1223.86	J/mol×K	1030.25	Joback Method
cpg	1238.49	J/mol×K	1067.43	Joback Method
cpg	1251.68	J/mol×K	1104.61	Joback Method
cpg	1263.48	J/mol×K	1141.79	Joback Method
cpg	1273.94	J/mol×K	1178.97	Joback Method
cpg	1283.10	J/mol×K	1216.15	Joback Method
dvisc	0.0002716	Pa×s	584.69	Joback Method

dvisc	0.0001441	Pa×s	652.75	Joback Method
dvisc	0.0000862	Pa×s	720.82	Joback Method
dvisc	0.0000563	Pa×s	788.88	Joback Method
dvisc	0.0000394	Pa×s	856.94	Joback Method
dvisc	0.0000290	Pa×s	925.01	Joback Method
dvisc	0.0000223	Pa×s	993.07	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=U393838&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

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