Pimelic acid, di(4-chloro-3-methylphenyl) ester

Inchi: InChI=1S/C21H22Cl2O4/c1-14-12-16(8-10-18(14)22)26-20(24)6-4-3-5-7-21(25)27-17-9-1
InchiKey: HGEXYUBYBWEILM-UHFFFAOYSA-N
Formula: C21H22Cl2O4
SMILES: Cc1cc(OC(=O)CCCCCC(=O)Oc2ccc(Cl)c(C)c2)ccc1Cl
Mol. weight [g/mol]: 409.30

Physical Properties

Property code	Value	Unit	Source
gf	-179.46	kJ/mol	Joback Method
hf	-570.67	kJ/mol	Joback Method
hfus	50.64	kJ/mol	Joback Method
hvap	96.62	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.072		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	980.60	K	Joback Method
tc	1213.72	K	Joback Method
tf	633.51	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.37	J/mol×K	980.60	Joback Method
cpg	890.52	J/mol×K	1019.45	Joback Method
cpg	900.32	J/mol×K	1058.31	Joback Method
cpg	908.79	J/mol×K	1097.16	Joback Method
cpg	915.97	J/mol×K	1136.01	Joback Method
cpg	921.87	J/mol×K	1174.86	Joback Method
cpg	926.54	J/mol×K	1213.72	Joback Method
dvisc	0.0002331	Pa×s	633.51	Joback Method

dvisc	0.0001522	Pa×s	691.36	Joback Method
dvisc	0.0001061	Pa×s	749.21	Joback Method
dvisc	0.0000779	Pa×s	807.05	Joback Method
dvisc	0.0000596	Pa×s	864.90	Joback Method
dvisc	0.0000472	Pa×s	922.75	Joback Method
dvisc	0.0000384	Pa×s	980.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416692&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