Pimelic acid, 4-chloro-3-methylphenyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C20H29ClO4/c1-14(2)12-16(4)24-19(22)8-6-5-7-9-20(23)25-17-10-11-18(21)15

InchiKey: VGQFSCLOXGCTOX-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: Cc1cc(OC(=O)CCCCCC(=O)OC(C)CC(C)C)ccc1Cl

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-273.98	kJ/mol	Joback Method
hf	-758.44	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.482		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2568.00		NIST Webbook
rinpol	2568.00		NIST Webbook
tb	882.77	K	Joback Method
tc	1092.15	K	Joback Method
tf	510.86	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.13	J/mol×K	882.77	Joback Method
cpg	920.19	J/mol×K	917.67	Joback Method
cpg	934.03	J/mol×K	952.56	Joback Method
cpg	946.67	J/mol×K	987.46	Joback Method
cpg	958.14	J/mol×K	1022.36	Joback Method
cpg	968.44	J/mol×K	1057.25	Joback Method
cpg	977.62	J/mol×K	1092.15	Joback Method
dvisc	0.0005211	Pa×s	510.86	Joback Method

dvisc	0.0002698	Pa×s	572.85	Joback Method
dvisc	0.0001588	Pa×s	634.83	Joback Method
dvisc	0.0001028	Pa×s	696.82	Joback Method
dvisc	0.0000714	Pa×s	758.80	Joback Method
dvisc	0.0000524	Pa×s	820.78	Joback Method
dvisc	0.0000402	Pa×s	882.77	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=U416684&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