Pimelic acid, 3,4-dichlorophenyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C19H26Cl2O4/c1-13(2)11-14(3)24-18(22)7-5-4-6-8-19(23)25-15-9-10-16(20)17

InchiKey: YGEFYFGIUUNNOJ-UHFFFAOYSA-N

Formula: C19H26Cl2O4

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 389.31

Physical Properties

Property code	Value	Unit	Source
gf	-294.33	kJ/mol	Joback Method
hf	-753.54	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	87.79	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.827		Crippen Method
mcvol	294.170	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	897.32	K	Joback Method
tc	1111.08	K	Joback Method
tf	529.51	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.48	J/mol×K	897.32	Joback Method
cpg	885.13	J/mol×K	932.95	Joback Method
cpg	897.59	J/mol×K	968.57	Joback Method
cpg	908.88	J/mol×K	1004.20	Joback Method
cpg	919.01	J/mol×K	1039.83	Joback Method
cpg	928.01	J/mol×K	1075.45	Joback Method
cpg	935.90	J/mol×K	1111.08	Joback Method
dvisc	0.0004670	Pa×s	529.51	Joback Method

dvisc	0.0002502	Pa×s	590.81	Joback Method
dvisc	0.0001507	Pa×s	652.11	Joback Method
dvisc	0.0000991	Pa×s	713.41	Joback Method
dvisc	0.0000696	Pa×s	774.72	Joback Method
dvisc	0.0000515	Pa×s	836.02	Joback Method
dvisc	0.0000397	Pa×s	897.32	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=U416731&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