Pimelic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi: InChI=1S/C18H25ClO4/c1-13(2)12-22-17(20)7-5-4-6-8-18(21)23-15-9-10-16(19)14(3)11-

InchiKey: PQWUDJIDINWULW-UHFFFAOYSA-N

Formula: C18H25ClO4

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

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-288.38	kJ/mol	Joback Method
hf	-711.88	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.704		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	837.45	K	Joback Method
tc	1044.56	K	Joback Method
tf	503.32	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.01	J/mol×K	837.45	Joback Method
cpg	802.59	J/mol×K	871.97	Joback Method
cpg	816.08	J/mol×K	906.49	Joback Method
cpg	828.48	J/mol×K	941.00	Joback Method
cpg	839.81	J/mol×K	975.52	Joback Method
cpg	850.09	J/mol×K	1010.04	Joback Method
cpg	859.32	J/mol×K	1044.56	Joback Method
dvisc	0.0005729	Pa×s	503.32	Joback Method

dvisc	0.0003239	Pa×s	559.01	Joback Method
dvisc	0.0002030	Pa×s	614.70	Joback Method
dvisc	0.0001375	Pa×s	670.38	Joback Method
dvisc	0.0000989	Pa×s	726.07	Joback Method
dvisc	0.0000745	Pa×s	781.76	Joback Method
dvisc	0.0000583	Pa×s	837.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416682&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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