Pimelic acid, di(2-chlorophenyl) ester

Inchi: InChI=1S/C19H18Cl2O4/c20-14-8-4-6-10-16(14)24-18(22)12-2-1-3-13-19(23)25-17-11-7
InchiKey: HNZJXPUYTUUEPG-UHFFFAOYSA-N
Formula: C19H18Cl2O4
SMILES: O=C(CCCCCC(=O)Oc1ccccc1Cl)Oc1ccccc1Cl
Mol. weight [g/mol]: 381.25

Physical Properties

Property code	Value	Unit	Source
gf	-177.04	kJ/mol	Joback Method
hf	-506.45	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.455		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	924.88	K	Joback Method
tc	1158.00	K	Joback Method
tf	585.93	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.42	J/mol×K	924.88	Joback Method
cpg	811.51	J/mol×K	1119.14	Joback Method
cpg	805.02	J/mol×K	1080.29	Joback Method
cpg	797.41	J/mol×K	1041.44	Joback Method
cpg	788.63	J/mol×K	1002.59	Joback Method
cpg	778.65	J/mol×K	963.73	Joback Method
cpg	816.89	J/mol×K	1158.00	Joback Method
dvisc	0.0000490	Pa×s	924.88	Joback Method

dvisc	0.0000611	Pa×s	868.39	Joback Method
dvisc	0.0000787	Pa×s	811.90	Joback Method
dvisc	0.0001051	Pa×s	755.40	Joback Method
dvisc	0.0001471	Pa×s	698.91	Joback Method
dvisc	0.0002184	Pa×s	642.42	Joback Method
dvisc	0.0003501	Pa×s	585.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416462&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