Pimelic acid, di(3,4-dichlorophenyl) ester

Inchi: InChI=1S/C19H16Cl4O4/c20-14-8-6-12(10-16(14)22)26-18(24)4-2-1-3-5-19(25)27-13-7-9
InchiKey: QZHBDCUOKURMRZ-UHFFFAOYSA-N
Formula: C19H16Cl4O4
SMILES: O=C(CCCCCC(=O)Oc1ccc(Cl)c(Cl)c1)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 450.14

Physical Properties

Property code	Value	Unit	Source
gf	-220.16	kJ/mol	Joback Method
hf	-560.87	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	100.94	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.762		Crippen Method
mcvol	294.890	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	3165.00		NIST Webbook
rinpol	3165.00		NIST Webbook
tb	1009.70	K	Joback Method
tc	1251.92	K	Joback Method
tf	670.81	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.65	J/mol×K	1009.70	Joback Method
cpg	808.94	J/mol×K	1050.07	Joback Method
cpg	815.96	J/mol×K	1090.44	Joback Method
cpg	821.73	J/mol×K	1130.81	Joback Method
cpg	826.28	J/mol×K	1171.18	Joback Method
cpg	829.65	J/mol×K	1211.55	Joback Method
cpg	831.86	J/mol×K	1251.92	Joback Method
dvisc	0.0002010	Pa×s	670.81	Joback Method

dvisc	0.0001359	Pa×s	727.29	Joback Method
dvisc	0.0000972	Pa×s	783.77	Joback Method
dvisc	0.0000727	Pa×s	840.26	Joback Method
dvisc	0.0000564	Pa×s	896.74	Joback Method
dvisc	0.0000451	Pa×s	953.22	Joback Method
dvisc	0.0000370	Pa×s	1009.70	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=U416740&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