Pimelic acid, 3,4-dichlorophenyl pentyl ester

Inchi: InChI=1S/C18H24Cl2O4/c1-2-3-7-12-23-17(21)8-5-4-6-9-18(22)24-14-10-11-15(19)16(20
InchiKey: UIHWCDDTOCKHQG-UHFFFAOYSA-N
Formula: C18H24Cl2O4
SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 375.29

Physical Properties

Property code	Value	Unit	Source
gf	-297.87	kJ/mol	Joback Method
hf	-722.34	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.583		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	875.32	K	Joback Method
tc	1084.97	K	Joback Method
tf	548.24	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.47	J/mol×K	875.32	Joback Method
cpg	868.21	J/mol×K	1050.03	Joback Method
cpg	859.16	J/mol×K	1015.09	Joback Method
cpg	849.09	J/mol×K	980.15	Joback Method
cpg	837.96	J/mol×K	945.20	Joback Method
cpg	825.76	J/mol×K	910.26	Joback Method
cpg	876.23	J/mol×K	1084.97	Joback Method
dvisc	0.0000549	Pa×s	875.32	Joback Method

dvisc	0.0000691	Pa×s	820.81	Joback Method
dvisc	0.0000897	Pa×s	766.29	Joback Method
dvisc	0.0001212	Pa×s	711.78	Joback Method
dvisc	0.0001723	Pa×s	657.27	Joback Method
dvisc	0.0002609	Pa×s	602.75	Joback Method
dvisc	0.0004290	Pa×s	548.24	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=U416732&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