Pimelic acid, 3,4-dichlorophenyl nonyl ester

Inchi: InChI=1S/C22H32Cl2O4/c1-2-3-4-5-6-7-11-16-27-21(25)12-9-8-10-13-22(26)28-18-14-15
InchiKey: SQZUYTDJYXVXJY-UHFFFAOYSA-N
Formula: C22H32Cl2O4
SMILES: CCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 431.39

Physical Properties

Property code	Value	Unit	Source
gf	-264.19	kJ/mol	Joback Method
hf	-804.90	kJ/mol	Joback Method
hfus	59.97	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.143		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	966.84	K	Joback Method
tc	1184.56	K	Joback Method
tf	593.32	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.35	J/mol×K	966.84	Joback Method
cpg	1106.10	J/mol×K	1148.27	Joback Method
cpg	1097.05	J/mol×K	1111.99	Joback Method
cpg	1086.79	J/mol×K	1075.70	Joback Method
cpg	1075.27	J/mol×K	1039.41	Joback Method
cpg	1062.47	J/mol×K	1003.13	Joback Method
cpg	1113.96	J/mol×K	1184.56	Joback Method
dvisc	0.0000304	Pa×s	966.84	Joback Method

dvisc	0.0000386	Pa×s	904.59	Joback Method
dvisc	0.0000510	Pa×s	842.33	Joback Method
dvisc	0.0000703	Pa×s	780.08	Joback Method
dvisc	0.0001025	Pa×s	717.83	Joback Method
dvisc	0.0001606	Pa×s	655.57	Joback Method
dvisc	0.0002763	Pa×s	593.32	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=U416736&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