1,2-Cyclohexanedicarboxylic acid, 2,5-dichlorophenyl octyl ester

Inchi: InChI=1S/C22H30Cl2O4/c1-2-3-4-5-6-9-14-27-21(25)17-10-7-8-11-18(17)22(26)28-20-15
InchiKey: QPMOYRSPZXFBCV-UHFFFAOYSA-N
Formula: C22H30Cl2O4
SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 429.38

Physical Properties

Property code	Value	Unit	Source
gf	-247.45	kJ/mol	Joback Method
hf	-770.92	kJ/mol	Joback Method
hfus	52.87	kJ/mol	Joback Method
hvap	95.37	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.609		Crippen Method
mcvol	325.580	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2928.00		NIST Webbook
tb	981.72	K	Joback Method
tc	1209.92	K	Joback Method
tf	596.46	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.21	J/mol×K	981.72	Joback Method
cpg	1059.97	J/mol×K	1019.75	Joback Method
cpg	1072.06	J/mol×K	1057.79	Joback Method
cpg	1082.51	J/mol×K	1095.82	Joback Method
cpg	1091.35	J/mol×K	1133.86	Joback Method
cpg	1098.62	J/mol×K	1171.89	Joback Method
cpg	1104.36	J/mol×K	1209.92	Joback Method
dvisc	0.0003592	Pa×s	596.46	Joback Method
dvisc	0.0002109	Pa×s	660.67	Joback Method

dvisc	0.0001361	Pa×s	724.88	Joback Method
dvisc	0.0000943	Pa×s	789.09	Joback Method
dvisc	0.0000690	Pa×s	853.30	Joback Method
dvisc	0.0000528	Pa×s	917.51	Joback Method
dvisc	0.0000418	Pa×s	981.72	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=U339803&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