Terephthalic acid, 2,2-dichloroethyl tridecyl ester

Inchi: InChI=1S/C23H34Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-17-28-22(26)19-13-15-20(16-14-19
InchiKey: XRBOFPLZFNMGFU-UHFFFAOYSA-N
Formula: C23H34Cl2O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]: 445.42

Physical Properties

Property code	Value	Unit	Source
gf	-248.58	kJ/mol	Joback Method
hf	-819.35	kJ/mol	Joback Method
hfus	59.42	kJ/mol	Joback Method
hvap	96.42	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.115		Crippen Method
mcvol	350.530	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	3158.00		NIST Webbook
rinpol	3158.00		NIST Webbook
tb	984.30	K	Joback Method
tc	1205.36	K	Joback Method
tf	577.07	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.16	J/mol×K	984.30	Joback Method
cpg	1168.90	J/mol×K	1168.52	Joback Method
cpg	1159.73	J/mol×K	1131.67	Joback Method
cpg	1149.31	J/mol×K	1094.83	Joback Method
cpg	1137.61	J/mol×K	1057.99	Joback Method
cpg	1124.57	J/mol×K	1021.14	Joback Method
cpg	1176.88	J/mol×K	1205.36	Joback Method
dvisc	0.0000231	Pa×s	984.30	Joback Method

dvisc	0.0000303	Pa×s	916.43	Joback Method
dvisc	0.0000414	Pa×s	848.56	Joback Method
dvisc	0.0000597	Pa×s	780.68	Joback Method
dvisc	0.0000923	Pa×s	712.81	Joback Method
dvisc	0.0001565	Pa×s	644.94	Joback Method
dvisc	0.0003004	Pa×s	577.07	Joback Method

Sources

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=U356252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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