Terephthalic acid, 2,2-dichloroethyl dodecyl ester

Inchi: InChI=1S/C22H32Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-16-27-21(25)18-12-14-19(15-13-18)22

InchiKey: SDMLVFVRZBURSU-UHFFFAOYSA-N

Formula: C22H32Cl2O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1

Mol. weight [g/mol]: 431.39

Physical Properties

Property code	Value	Unit	Source
gf	-257.00	kJ/mol	Joback Method
hf	-798.71	kJ/mol	Joback Method
hfus	56.83	kJ/mol	Joback Method
hvap	94.20	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.725		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	961.42	K	Joback Method
tc	1178.64	K	Joback Method
tf	565.80	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.78	J/mol×K	961.42	Joback Method
cpg	1063.99	J/mol×K	997.62	Joback Method
cpg	1076.90	J/mol×K	1033.83	Joback Method
cpg	1088.54	J/mol×K	1070.03	Joback Method
cpg	1098.95	J/mol×K	1106.23	Joback Method
cpg	1108.17	J/mol×K	1142.44	Joback Method
cpg	1116.24	J/mol×K	1178.64	Joback Method
dvisc	0.0003401	Pa×s	565.80	Joback Method

dvisc	0.0001789	Pa×s	631.74	Joback Method
dvisc	0.0001063	Pa×s	697.67	Joback Method
dvisc	0.0000691	Pa×s	763.61	Joback Method
dvisc	0.0000481	Pa×s	829.55	Joback Method
dvisc	0.0000353	Pa×s	895.48	Joback Method
dvisc	0.0000270	Pa×s	961.42	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=U356251&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

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