Terephthalic acid, 2,2-dichloroethyl tetradecyl ester

Inchi: InChI=1S/C24H36Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-29-23(27)20-14-16-21(17-15

InchiKey: RIJPEXVOIRXCDZ-UHFFFAOYSA-N

Formula: C24H36Cl2O4

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

Mol. weight [g/mol]: 459.45

Physical Properties

Property code	Value	Unit	Source
gf	-240.16	kJ/mol	Joback Method
hf	-839.99	kJ/mol	Joback Method
hfus	62.01	kJ/mol	Joback Method
hvap	98.65	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.505		Crippen Method
mcvol	364.620	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	3262.00		NIST Webbook
rinpol	3262.00		NIST Webbook
tb	1007.18	K	Joback Method
tc	1233.10	K	Joback Method
tf	588.34	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.02	J/mol×K	1007.18	Joback Method
cpg	1185.65	J/mol×K	1044.83	Joback Method
cpg	1198.81	J/mol×K	1082.49	Joback Method
cpg	1210.57	J/mol×K	1120.14	Joback Method
cpg	1220.98	J/mol×K	1157.80	Joback Method
cpg	1230.09	J/mol×K	1195.45	Joback Method
cpg	1237.96	J/mol×K	1233.10	Joback Method
dvisc	0.0002647	Pa×s	588.34	Joback Method

dvisc	0.0001366	Pa×s	658.15	Joback Method
dvisc	0.0000800	Pa×s	727.95	Joback Method
dvisc	0.0000515	Pa×s	797.76	Joback Method
dvisc	0.0000356	Pa×s	867.57	Joback Method
dvisc	0.0000259	Pa×s	937.37	Joback Method
dvisc	0.0000198	Pa×s	1007.18	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=U356253&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