Terephthalic acid, 2,2-dichloroethyl hexyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-2-3-4-5-10-21-15(19)12-6-8-13(9-7-12)16(20)22-11-14(17)18

InchiKey: PLWSOSCJUKVFBC-UHFFFAOYSA-N

Formula: C16H20Cl2O4

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

Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-307.52	kJ/mol	Joback Method
hf	-674.87	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.384		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2431.00		NIST Webbook
tb	824.14	K	Joback Method
tc	1036.24	K	Joback Method
tf	498.18	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.68	J/mol×K	824.14	Joback Method
cpg	713.70	J/mol×K	859.49	Joback Method
cpg	725.67	J/mol×K	894.84	Joback Method
cpg	736.63	J/mol×K	930.19	Joback Method
cpg	746.58	J/mol×K	965.54	Joback Method
cpg	755.55	J/mol×K	1000.89	Joback Method
cpg	763.55	J/mol×K	1036.24	Joback Method
dvisc	0.0006699	Pa×s	498.18	Joback Method
dvisc	0.0003768	Pa×s	552.51	Joback Method

dvisc	0.0002349	Pa×s	606.83	Joback Method
dvisc	0.0001583	Pa×s	661.16	Joback Method
dvisc	0.0001132	Pa×s	715.49	Joback Method
dvisc	0.0000849	Pa×s	769.81	Joback Method
dvisc	0.0000662	Pa×s	824.14	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=U356246&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