Terephthalic acid, 2-chloropropyl hexyl ester

Inchi: InChI=1S/C17H23ClO4/c1-3-4-5-6-11-21-16(19)14-7-9-15(10-8-14)17(20)22-12-13(2)18/
InchiKey: JRNSUEZMONBKGI-UHFFFAOYSA-N
Formula: C17H23ClO4
SMILES: CCCCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-287.17	kJ/mol	Joback Method
hf	-679.77	kJ/mol	Joback Method
hfus	39.69	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.208		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2371.00		NIST Webbook
tb	809.59	K	Joback Method
tc	1016.62	K	Joback Method
tf	479.53	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.89	J/mol×K	809.59	Joback Method
cpg	793.70	J/mol×K	982.11	Joback Method
cpg	783.39	J/mol×K	947.61	Joback Method
cpg	772.07	J/mol×K	913.10	Joback Method
cpg	759.73	J/mol×K	878.60	Joback Method
cpg	746.34	J/mol×K	844.09	Joback Method
cpg	803.02	J/mol×K	1016.62	Joback Method
dvisc	0.0000663	Pa×s	809.59	Joback Method
dvisc	0.0000857	Pa×s	754.58	Joback Method

dvisc	0.0001151	Pa×s	699.57	Joback Method
dvisc	0.0001628	Pa×s	644.56	Joback Method
dvisc	0.0002455	Pa×s	589.55	Joback Method
dvisc	0.0004031	Pa×s	534.54	Joback Method
dvisc	0.0007413	Pa×s	479.53	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=U356172&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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