Isophthalic acid, 2-chloropropyl isohexyl ester

Inchi: InChI=1S/C17H23ClO4/c1-12(2)6-5-9-21-16(19)14-7-4-8-15(10-14)17(20)22-11-13(3)18/
InchiKey: MNSSVASRGLFGDM-UHFFFAOYSA-N
Formula: C17H23ClO4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OCC(C)Cl)c1
Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-289.61	kJ/mol	Joback Method
hf	-685.05	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.064		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
tb	809.15	K	Joback Method
tc	1018.80	K	Joback Method
tf	464.53	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.45	J/mol×K	809.15	Joback Method
cpg	794.77	J/mol×K	983.86	Joback Method
cpg	784.43	J/mol×K	948.92	Joback Method
cpg	773.05	J/mol×K	913.98	Joback Method
cpg	760.60	J/mol×K	879.03	Joback Method
cpg	747.08	J/mol×K	844.09	Joback Method
cpg	804.08	J/mol×K	1018.80	Joback Method
dvisc	0.0000609	Pa×s	809.15	Joback Method

dvisc	0.0000799	Pa×s	751.71	Joback Method
dvisc	0.0001097	Pa×s	694.28	Joback Method
dvisc	0.0001594	Pa×s	636.84	Joback Method
dvisc	0.0002494	Pa×s	579.40	Joback Method
dvisc	0.0004307	Pa×s	521.97	Joback Method
dvisc	0.0008514	Pa×s	464.53	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=U356359&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