Isophthalic acid, propyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H13Cl3O4/c1-2-6-23-16(21)10-4-3-5-11(7-10)17(22)24-15-13(19)8-12(18)9

InchiKey: CANZSVFEHFESDK-UHFFFAOYSA-N

Formula: C17H13Cl3O4

SMILES: CCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cc(Cl)cc2Cl)c1

Mol. weight [g/mol]: 387.64

Physical Properties

Property code	Value	Unit	Source
gf	-225.07	kJ/mol	Joback Method
hf	-503.85	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.433		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	926.51	K	Joback Method
tc	1168.45	K	Joback Method
tf	618.35	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.85	J/mol×K	926.51	Joback Method
cpg	705.65	J/mol×K	1128.13	Joback Method
cpg	701.07	J/mol×K	1087.81	Joback Method
cpg	695.31	J/mol×K	1047.48	Joback Method
cpg	688.37	J/mol×K	1007.16	Joback Method
cpg	680.22	J/mol×K	966.83	Joback Method
cpg	709.08	J/mol×K	1168.45	Joback Method
dvisc	0.0000583	Pa×s	926.51	Joback Method

dvisc	0.0000706	Pa×s	875.15	Joback Method
dvisc	0.0000876	Pa×s	823.79	Joback Method
dvisc	0.0001118	Pa×s	772.43	Joback Method
dvisc	0.0001478	Pa×s	721.07	Joback Method
dvisc	0.0002038	Pa×s	669.71	Joback Method
dvisc	0.0002965	Pa×s	618.35	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=U344566&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