Isophthalic acid, 2-chloro-5-methylphenyl propyl ester

Inchi: InChI=1S/C18H17ClO4/c1-3-9-22-17(20)13-5-4-6-14(11-13)18(21)23-16-10-12(2)7-8-15(

InchiKey: BKUDKOHFBCNLCN-UHFFFAOYSA-N

Formula: C18H17ClO4

SMILES: CCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2Cl)c1

Mol. weight [g/mol]: 332.78

Physical Properties

Property code	Value	Unit	Source
gf	-183.16	kJ/mol	Joback Method
hf	-481.54	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.434		Crippen Method
mcvol	244.080	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2552.00		NIST Webbook
tb	869.55	K	Joback Method
tc	1102.44	K	Joback Method
tf	557.26	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.43	J/mol×K	869.55	Joback Method
cpg	700.80	J/mol×K	908.37	Joback Method
cpg	711.92	J/mol×K	947.18	Joback Method
cpg	721.82	J/mol×K	986.00	Joback Method
cpg	730.53	J/mol×K	1024.81	Joback Method
cpg	738.05	J/mol×K	1063.63	Joback Method
cpg	744.41	J/mol×K	1102.44	Joback Method
dvisc	0.0004102	Pa×s	557.26	Joback Method
dvisc	0.0002660	Pa×s	609.31	Joback Method

dvisc	0.0001846	Pa×s	661.36	Joback Method
dvisc	0.0001352	Pa×s	713.40	Joback Method
dvisc	0.0001033	Pa×s	765.45	Joback Method
dvisc	0.0000816	Pa×s	817.50	Joback Method
dvisc	0.0000664	Pa×s	869.55	Joback Method

Sources

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=U356563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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