Isophthalic acid, 3-chlorophenyl ethyl ester

Inchi: InChI=1S/C16H13ClO4/c1-2-20-15(18)11-5-3-6-12(9-11)16(19)21-14-8-4-7-13(17)10-14/
InchiKey: FLARZRNEIVBXLS-UHFFFAOYSA-N
Formula: C16H13ClO4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2)c1
Mol. weight [g/mol]: 304.73

Physical Properties

Property code	Value	Unit	Source
gf	-190.37	kJ/mol	Joback Method
hf	-428.79	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.736		Crippen Method
mcvol	215.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	818.81	K	Joback Method
tc	1057.73	K	Joback Method
tf	522.20	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.61	J/mol×K	818.81	Joback Method
cpg	591.66	J/mol×K	858.63	Joback Method
cpg	602.52	J/mol×K	898.45	Joback Method
cpg	612.21	J/mol×K	938.27	Joback Method
cpg	620.74	J/mol×K	978.09	Joback Method
cpg	628.16	J/mol×K	1017.91	Joback Method
cpg	634.47	J/mol×K	1057.73	Joback Method
dvisc	0.0005504	Pa×s	522.20	Joback Method

dvisc	0.0003526	Pa×s	571.63	Joback Method
dvisc	0.0002425	Pa×s	621.07	Joback Method
dvisc	0.0001762	Pa×s	670.50	Joback Method
dvisc	0.0001338	Pa×s	719.94	Joback Method
dvisc	0.0001052	Pa×s	769.38	Joback Method
dvisc	0.0000852	Pa×s	818.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344599&Units=SI
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

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