Isophthalic acid, 2-chlorophenyl propyl ester

Inchi: InChI=1S/C17H15ClO4/c1-2-10-21-16(19)12-6-5-7-13(11-12)17(20)22-15-9-4-3-8-14(15)
InchiKey: MQMYUJAUXCMFEE-UHFFFAOYSA-N
Formula: C17H15ClO4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccccc2Cl)c1
Mol. weight [g/mol]: 318.75

Physical Properties

Property code	Value	Unit	Source
gf	-181.95	kJ/mol	Joback Method
hf	-449.43	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	82.01	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.126		Crippen Method
mcvol	229.990	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	841.69	K	Joback Method
tc	1076.92	K	Joback Method
tf	533.47	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.29	J/mol×K	841.69	Joback Method
cpg	683.82	J/mol×K	1037.71	Joback Method
cpg	676.24	J/mol×K	998.51	Joback Method
cpg	667.53	J/mol×K	959.30	Joback Method
cpg	657.64	J/mol×K	920.10	Joback Method
cpg	646.57	J/mol×K	880.89	Joback Method
cpg	690.29	J/mol×K	1076.92	Joback Method
dvisc	0.0000747	Pa×s	841.69	Joback Method

dvisc	0.0000926	Pa×s	790.32	Joback Method
dvisc	0.0001183	Pa×s	738.95	Joback Method
dvisc	0.0001568	Pa×s	687.58	Joback Method
dvisc	0.0002174	Pa×s	636.21	Joback Method
dvisc	0.0003193	Pa×s	584.84	Joback Method
dvisc	0.0005049	Pa×s	533.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344496&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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