Isophthalic acid, 4-chlorophenyl hexyl ester

Inchi: InChI=1S/C20H21ClO4/c1-2-3-4-5-13-24-19(22)15-7-6-8-16(14-15)20(23)25-18-11-9-17(
InchiKey: FQVJJBSXQTZVEA-UHFFFAOYSA-N
Formula: C20H21ClO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 360.83

Physical Properties

Property code	Value	Unit	Source
gf	-156.69	kJ/mol	Joback Method
hf	-511.35	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	88.69	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.296		Crippen Method
mcvol	272.260	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2889.00		NIST Webbook
rinpol	2889.00		NIST Webbook
tb	910.33	K	Joback Method
tc	1138.42	K	Joback Method
tf	567.28	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.40	J/mol×K	910.33	Joback Method
cpg	816.11	J/mol×K	948.34	Joback Method
cpg	827.53	J/mol×K	986.36	Joback Method
cpg	837.71	J/mol×K	1024.37	Joback Method
cpg	846.69	J/mol×K	1062.39	Joback Method
cpg	854.49	J/mol×K	1100.40	Joback Method
cpg	861.16	J/mol×K	1138.42	Joback Method
dvisc	0.0003793	Pa×s	567.28	Joback Method

dvisc	0.0002313	Pa×s	624.46	Joback Method
dvisc	0.0001532	Pa×s	681.63	Joback Method
dvisc	0.0001082	Pa×s	738.81	Joback Method
dvisc	0.0000803	Pa×s	795.98	Joback Method
dvisc	0.0000620	Pa×s	853.15	Joback Method
dvisc	0.0000495	Pa×s	910.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344581&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