Isophthalic acid, 4-chloro-3-methylphenyl isohexyl ester

Inchi: InChI=1S/C21H23ClO4/c1-14(2)6-5-11-25-20(23)16-7-4-8-17(13-16)21(24)26-18-9-10-19

InchiKey: NJACJGXKEZMQIY-UHFFFAOYSA-N

Formula: C21H23ClO4

SMILES: Cc1cc(OC(=O)c2cccc(C(=O)OCCCC(C)C)c2)ccc1Cl

Mol. weight [g/mol]: 374.86

Physical Properties

Property code	Value	Unit	Source
gf	-160.34	kJ/mol	Joback Method
hf	-548.74	kJ/mol	Joback Method
hfus	43.31	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.461		Crippen Method
mcvol	286.350	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook
tb	937.75	K	Joback Method
tc	1168.01	K	Joback Method
tf	576.07	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.43	J/mol×K	937.75	Joback Method
cpg	873.18	J/mol×K	976.13	Joback Method
cpg	884.55	J/mol×K	1014.50	Joback Method
cpg	894.60	J/mol×K	1052.88	Joback Method
cpg	903.35	J/mol×K	1091.26	Joback Method
cpg	910.82	J/mol×K	1129.64	Joback Method
cpg	917.06	J/mol×K	1168.01	Joback Method
dvisc	0.0003287	Pa×s	576.07	Joback Method

dvisc	0.0001959	Pa×s	636.35	Joback Method
dvisc	0.0001277	Pa×s	696.63	Joback Method
dvisc	0.0000891	Pa×s	756.91	Joback Method
dvisc	0.0000656	Pa×s	817.19	Joback Method
dvisc	0.0000504	Pa×s	877.47	Joback Method
dvisc	0.0000400	Pa×s	937.75	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=U344593&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