Isophthalic acid, (2-chlorocyclohexyl)methyl pentyl ester

Inchi: InChI=1S/C20H27ClO4/c1-2-3-6-12-24-19(22)15-9-7-10-16(13-15)20(23)25-14-17-8-4-5-

InchiKey: NJQIUCFJYPWOMA-UHFFFAOYSA-N

Formula: C20H27ClO4

SMILES: CCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2Cl)c1

Mol. weight [g/mol]: 366.88

Physical Properties

Property code	Value	Unit	Source
gf	-242.73	kJ/mol	Joback Method
hf	-702.43	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	85.87	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.988		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	893.55	K	Joback Method
tc	1116.35	K	Joback Method
tf	531.48	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.66	J/mol×K	893.55	Joback Method
cpg	919.39	J/mol×K	930.68	Joback Method
cpg	933.57	J/mol×K	967.82	Joback Method
cpg	946.22	J/mol×K	1004.95	Joback Method
cpg	957.38	J/mol×K	1042.08	Joback Method
cpg	967.07	J/mol×K	1079.22	Joback Method
cpg	975.31	J/mol×K	1116.35	Joback Method
dvisc	0.0006106	Pa×s	531.48	Joback Method

dvisc	0.0003460	Pa×s	591.83	Joback Method
dvisc	0.0002178	Pa×s	652.17	Joback Method
dvisc	0.0001483	Pa×s	712.51	Joback Method
dvisc	0.0001072	Pa×s	772.86	Joback Method
dvisc	0.0000812	Pa×s	833.20	Joback Method
dvisc	0.0000639	Pa×s	893.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343795&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