Isophthalic acid, isohexyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C20H19Cl3O4/c1-12(2)5-4-8-26-19(24)13-6-3-7-14(9-13)20(25)27-18-11-16(22
InchiKey: PGYYHQREOVXUTR-UHFFFAOYSA-N
Formula: C20H19Cl3O4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)c1
Mol. weight [g/mol]: 429.72

Physical Properties

Property code	Value	Unit	Source
gf	-202.25	kJ/mol	Joback Method
hf	-571.05	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.459		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	3053.00		NIST Webbook
rinpol	3053.00		NIST Webbook
tb	994.71	K	Joback Method
tc	1234.50	K	Joback Method
tf	637.16	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.96	J/mol×K	994.71	Joback Method
cpg	876.35	J/mol×K	1194.53	Joback Method
cpg	871.87	J/mol×K	1154.57	Joback Method
cpg	866.11	J/mol×K	1114.60	Joback Method
cpg	859.06	J/mol×K	1074.64	Joback Method
cpg	850.69	J/mol×K	1034.67	Joback Method
cpg	879.60	J/mol×K	1234.50	Joback Method
dvisc	0.0000343	Pa×s	994.71	Joback Method

dvisc	0.0000425	Pa×s	935.12	Joback Method
dvisc	0.0000543	Pa×s	875.53	Joback Method
dvisc	0.0000717	Pa×s	815.93	Joback Method
dvisc	0.0000991	Pa×s	756.34	Joback Method
dvisc	0.0001446	Pa×s	696.75	Joback Method
dvisc	0.0002265	Pa×s	637.16	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=U356612&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