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

Inchi: InChI=1S/C23H25Cl3O4/c1-2-3-4-5-6-7-8-12-29-22(27)16-10-9-11-17(13-16)23(28)30-21
InchiKey: WXQPGMBBBFACRI-UHFFFAOYSA-N
Formula: C23H25Cl3O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)c1
Mol. weight [g/mol]: 471.80

Physical Properties

Property code	Value	Unit	Source
gf	-174.55	kJ/mol	Joback Method
hf	-627.69	kJ/mol	Joback Method
hfus	60.02	kJ/mol	Joback Method
hvap	105.46	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	7.773		Crippen Method
mcvol	339.010	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	3412.00		NIST Webbook
rinpol	3412.00		NIST Webbook
tb	1063.79	K	Joback Method
tc	1305.08	K	Joback Method
tf	685.97	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.27	J/mol×K	1063.79	Joback Method
cpg	1025.13	J/mol×K	1104.00	Joback Method
cpg	1033.53	J/mol×K	1144.22	Joback Method
cpg	1040.53	J/mol×K	1184.43	Joback Method
cpg	1046.17	J/mol×K	1224.65	Joback Method
cpg	1050.49	J/mol×K	1264.86	Joback Method
cpg	1053.53	J/mol×K	1305.08	Joback Method
dvisc	0.0001539	Pa×s	685.97	Joback Method

dvisc	0.0000991	Pa×s	748.94	Joback Method
dvisc	0.0000684	Pa×s	811.91	Joback Method
dvisc	0.0000497	Pa×s	874.88	Joback Method
dvisc	0.0000378	Pa×s	937.85	Joback Method
dvisc	0.0000297	Pa×s	1000.82	Joback Method
dvisc	0.0000240	Pa×s	1063.79	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=U356616&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