

Isophthalic acid, nonyl 2,4,6-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)30-2
InchiKey:	AAXXQKUSRGISMD-UHFFFAOYSA-N
Formula:	C23H25Cl3O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cc(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	3413.00		NIST Webbook
rinpol	3413.00		NIST Webbook
tb	1063.79	K	Joback Method
tc	1305.08	K	Joback Method
tf	685.97	K	Joback Method
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.27	J/molxK	1063.79	Joback Method
cpg	1050.49	J/molxK	1264.86	Joback Method
cpg	1046.17	J/molxK	1224.65	Joback Method
cpg	1040.53	J/molxK	1184.43	Joback Method
cpg	1033.53	J/molxK	1144.22	Joback Method
cpg	1025.13	J/molxK	1104.00	Joback Method
cpg	1053.53	J/molxK	1305.08	Joback Method
dvisc	0.0000240	Paxs	1063.79	Joback Method

dvisc	0.0000297	Paxs	1000.82	Joback Method
dvisc	0.0000378	Paxs	937.85	Joback Method
dvisc	0.0000497	Paxs	874.88	Joback Method
dvisc	0.0000684	Paxs	811.91	Joback Method
dvisc	0.0000991	Paxs	748.94	Joback Method
dvisc	0.0001539	Paxs	685.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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