Isophthalic acid, 4-chlorophenyl nonyl ester

Inchi: InChI=1S/C23H27ClO4/c1-2-3-4-5-6-7-8-16-27-22(25)18-10-9-11-19(17-18)23(26)28-21-
InchiKey: WDOCLFDVMZZEMW-UHFFFAOYSA-N
Formula: C23H27ClO4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 402.91

Physical Properties

Property code	Value	Unit	Source
gf	-131.43	kJ/mol	Joback Method
hf	-573.27	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	95.37	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	6.467		Crippen Method
mcvol	314.530	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	3222.00		NIST Webbook
rinpol	3222.00		NIST Webbook
tb	978.97	K	Joback Method
tc	1206.69	K	Joback Method
tf	601.09	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.77	J/mol×K	978.97	Joback Method
cpg	1030.12	J/mol×K	1168.74	Joback Method
cpg	1022.39	J/mol×K	1130.78	Joback Method
cpg	1013.44	J/mol×K	1092.83	Joback Method
cpg	1003.22	J/mol×K	1054.88	Joback Method
cpg	991.68	J/mol×K	1016.92	Joback Method
cpg	1036.67	J/mol×K	1206.69	Joback Method
dvisc	0.0000321	Pa×s	978.97	Joback Method

dvisc	0.0000406	Pa×s	915.99	Joback Method
dvisc	0.0000531	Pa×s	853.01	Joback Method
dvisc	0.0000726	Pa×s	790.03	Joback Method
dvisc	0.0001049	Pa×s	727.05	Joback Method
dvisc	0.0001623	Pa×s	664.07	Joback Method
dvisc	0.0002752	Pa×s	601.09	Joback Method

Sources

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=U344584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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