Isophthalic acid, 2,6-dichlorophenyl nonyl ester

Inchi: InChI=1S/C23H26Cl2O4/c1-2-3-4-5-6-7-8-15-28-22(26)17-11-9-12-18(16-17)23(27)29-21

InchiKey: QSJLDNWWBMMFPX-UHFFFAOYSA-N

Formula: C23H26Cl2O4

SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1

Mol. weight [g/mol]: 437.36

Physical Properties

Property code	Value	Unit	Source
gf	-152.99	kJ/mol	Joback Method
hf	-600.48	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	100.41	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.120		Crippen Method
mcvol	326.770	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	3278.00		NIST Webbook
rinpol	3278.00		NIST Webbook
tb	1021.38	K	Joback Method
tc	1255.57	K	Joback Method
tf	643.53	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.18	J/mol×K	1021.38	Joback Method
cpg	1041.66	J/mol×K	1216.54	Joback Method
cpg	1035.58	J/mol×K	1177.51	Joback Method
cpg	1028.24	J/mol×K	1138.48	Joback Method
cpg	1019.59	J/mol×K	1099.44	Joback Method
cpg	1009.59	J/mol×K	1060.41	Joback Method
cpg	1046.53	J/mol×K	1255.57	Joback Method
dvisc	0.0000278	Pa×s	1021.38	Joback Method

dvisc	0.0000348	Pa×s	958.40	Joback Method
dvisc	0.0000448	Pa×s	895.43	Joback Method
dvisc	0.0000601	Pa×s	832.45	Joback Method
dvisc	0.0000845	Pa×s	769.48	Joback Method
dvisc	0.0001263	Pa×s	706.50	Joback Method
dvisc	0.0002042	Pa×s	643.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344627&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