Isophthalic acid, monochloride, 2-methylcyclohexyl ester

Inchi: InChI=1S/C15H17ClO3/c1-10-5-2-3-8-13(10)19-15(18)12-7-4-6-11(9-12)14(16)17/h4,6-7

InchiKey: QMIRDWFKWIOXMX-UHFFFAOYSA-N

Formula: C15H17ClO3

SMILES: CC1CCCCC1OC(=O)c1cccc(C(=O)Cl)c1

Mol. weight [g/mol]: 280.75

Physical Properties

Property code	Value	Unit	Source
gf	-179.83	kJ/mol	Joback Method
hf	-467.01	kJ/mol	Joback Method
hfus	29.75	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.801		Crippen Method
mcvol	208.840	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	756.73	K	Joback Method
tc	996.30	K	Joback Method
tf	452.90	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.41	J/mol×K	756.73	Joback Method
cpg	605.87	J/mol×K	796.66	Joback Method
cpg	620.91	J/mol×K	836.59	Joback Method
cpg	634.54	J/mol×K	876.51	Joback Method
cpg	646.80	J/mol×K	916.44	Joback Method
cpg	657.72	J/mol×K	956.37	Joback Method
cpg	667.34	J/mol×K	996.30	Joback Method
dvisc	0.0013196	Pa×s	452.90	Joback Method

dvisc	0.0007801	Pa×s	503.54	Joback Method
dvisc	0.0005077	Pa×s	554.18	Joback Method
dvisc	0.0003550	Pa×s	604.82	Joback Method
dvisc	0.0002624	Pa×s	655.45	Joback Method
dvisc	0.0002025	Pa×s	706.09	Joback Method
dvisc	0.0001618	Pa×s	756.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345758&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