Isophthalic acid, monochloride, hexyl ester

Inchi: InChI=1S/C14H17ClO3/c1-2-3-4-5-9-18-14(17)12-8-6-7-11(10-12)13(15)16/h6-8,10H,2-5
InchiKey: BIOOGHNAZHAIJW-UHFFFAOYSA-N
Formula: C14H17ClO3
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Cl)c1
Mol. weight [g/mol]: 268.74

Physical Properties

Property code	Value	Unit	Source
gf	-204.99	kJ/mol	Joback Method
hf	-480.35	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.803		Crippen Method
mcvol	205.610	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	718.97	K	Joback Method
tc	930.05	K	Joback Method
tf	438.49	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.87	J/mol×K	718.97	Joback Method
cpg	553.50	J/mol×K	754.15	Joback Method
cpg	566.23	J/mol×K	789.33	Joback Method
cpg	578.07	J/mol×K	824.51	Joback Method
cpg	589.06	J/mol×K	859.69	Joback Method
cpg	599.22	J/mol×K	894.87	Joback Method
cpg	608.57	J/mol×K	930.05	Joback Method
dvisc	0.0011819	Pa×s	438.49	Joback Method

dvisc	0.0006981	Pa×s	485.24	Joback Method
dvisc	0.0004523	Pa×s	531.98	Joback Method
dvisc	0.0003143	Pa×s	578.73	Joback Method
dvisc	0.0002307	Pa×s	625.48	Joback Method
dvisc	0.0001767	Pa×s	672.22	Joback Method
dvisc	0.0001401	Pa×s	718.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344716&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