Isophthalic acid, (2-chlorocyclohexyl)methyl isobutyl ester

Inchi: InChI=1S/C19H25ClO4/c1-13(2)11-23-18(21)14-7-5-8-15(10-14)19(22)24-12-16-6-3-4-9-

InchiKey: QGDAVLARXSUQOA-UHFFFAOYSA-N

Formula: C19H25ClO4

SMILES: CC(C)COC(=O)c1cccc(C(=O)OCC2CCCCC2Cl)c1

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-253.59	kJ/mol	Joback Method
hf	-687.07	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.454		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	870.23	K	Joback Method
tc	1097.35	K	Joback Method
tf	505.21	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.28	J/mol×K	870.23	Joback Method
cpg	909.68	J/mol×K	1059.50	Joback Method
cpg	899.86	J/mol×K	1021.64	Joback Method
cpg	888.54	J/mol×K	983.79	Joback Method
cpg	875.68	J/mol×K	945.94	Joback Method
cpg	861.27	J/mol×K	908.08	Joback Method
cpg	918.01	J/mol×K	1097.35	Joback Method
dvisc	0.0000672	Pa×s	870.23	Joback Method

dvisc	0.0000863	Pa×s	809.39	Joback Method
dvisc	0.0001156	Pa×s	748.56	Joback Method
dvisc	0.0001629	Pa×s	687.72	Joback Method
dvisc	0.0002454	Pa×s	626.88	Joback Method
dvisc	0.0004037	Pa×s	566.05	Joback Method
dvisc	0.0007488	Pa×s	505.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343794&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