Isophthalic acid, 2-chloro-5-methylphenyl isobutyl ester

Inchi: InChI=1S/C19H19ClO4/c1-12(2)11-23-18(21)14-5-4-6-15(10-14)19(22)24-17-9-13(3)7-8-

InchiKey: BXDMZRTXAICUAB-UHFFFAOYSA-N

Formula: C19H19ClO4

SMILES: Cc1ccc(Cl)c(OC(=O)c2cccc(C(=O)OCC(C)C)c2)c1

Mol. weight [g/mol]: 346.81

Physical Properties

Property code	Value	Unit	Source
gf	-177.18	kJ/mol	Joback Method
hf	-507.46	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.680		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2598.00		NIST Webbook
tb	891.99	K	Joback Method
tc	1125.54	K	Joback Method
tf	553.53	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.42	J/mol×K	891.99	Joback Method
cpg	758.05	J/mol×K	930.91	Joback Method
cpg	769.36	J/mol×K	969.84	Joback Method
cpg	779.38	J/mol×K	1008.76	Joback Method
cpg	788.13	J/mol×K	1047.69	Joback Method
cpg	795.64	J/mol×K	1086.61	Joback Method
cpg	801.95	J/mol×K	1125.54	Joback Method
dvisc	0.0004025	Pa×s	553.53	Joback Method
dvisc	0.0002455	Pa×s	609.94	Joback Method

dvisc	0.0001628	Pa×s	666.35	Joback Method
dvisc	0.0001152	Pa×s	722.76	Joback Method
dvisc	0.0000856	Pa×s	779.17	Joback Method
dvisc	0.0000663	Pa×s	835.58	Joback Method
dvisc	0.0000530	Pa×s	891.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356564&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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