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

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

InchiKey: XFJDAEGOVRLVDT-UHFFFAOYSA-N

Formula: C19H19ClO4

SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2Cl)c1

Mol. weight [g/mol]: 346.81

Physical Properties

Property code	Value	Unit	Source
gf	-174.74	kJ/mol	Joback Method
hf	-502.18	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.825		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2649.00		NIST Webbook
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tb	892.43	K	Joback Method
tc	1122.94	K	Joback Method
tf	568.53	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.88	J/mol×K	892.43	Joback Method
cpg	757.38	J/mol×K	930.85	Joback Method
cpg	768.61	J/mol×K	969.27	Joback Method
cpg	778.59	J/mol×K	1007.69	Joback Method
cpg	787.36	J/mol×K	1046.11	Joback Method
cpg	794.94	J/mol×K	1084.52	Joback Method
cpg	801.34	J/mol×K	1122.94	Joback Method
dvisc	0.0003739	Pa×s	568.53	Joback Method

dvisc	0.0002395	Pa×s	622.51	Joback Method
dvisc	0.0001647	Pa×s	676.50	Joback Method
dvisc	0.0001197	Pa×s	730.48	Joback Method
dvisc	0.0000909	Pa×s	784.46	Joback Method
dvisc	0.0000716	Pa×s	838.45	Joback Method
dvisc	0.0000580	Pa×s	892.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356565&Units=SI

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