1,2-Cyclohexanedicarboxylic acid, butyl 3-chlorophenyl ester

Inchi: InChI=1S/C18H23ClO4/c1-2-3-11-22-17(20)15-9-4-5-10-16(15)18(21)23-14-8-6-7-13(19)

InchiKey: XAJFXAAMXAZOMM-UHFFFAOYSA-N

Formula: C18H23ClO4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-259.57	kJ/mol	Joback Method
hf	-661.15	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.395		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
tb	847.79	K	Joback Method
tc	1074.08	K	Joback Method
tf	508.94	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.53	J/mol×K	847.79	Joback Method
cpg	851.03	J/mol×K	1036.37	Joback Method
cpg	841.06	J/mol×K	998.65	Joback Method
cpg	829.65	J/mol×K	960.94	Joback Method
cpg	816.77	J/mol×K	923.22	Joback Method
cpg	802.40	J/mol×K	885.51	Joback Method
cpg	859.58	J/mol×K	1074.08	Joback Method
dvisc	0.0000842	Pa×s	847.79	Joback Method
dvisc	0.0001063	Pa×s	791.32	Joback Method
dvisc	0.0001391	Pa×s	734.84	Joback Method

dvisc	0.0001904	Pa×s	678.37	Joback Method
dvisc	0.0002760	Pa×s	621.89	Joback Method
dvisc	0.0004307	Pa×s	565.41	Joback Method
dvisc	0.0007421	Pa×s	508.94	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=R465399&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume