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

Inchi: InChI=1S/C18H22Cl2O4/c1-2-3-11-23-17(21)12-7-4-5-8-13(12)18(22)24-15-10-6-9-14(19

InchiKey: UWFRKKNUPXASQX-UHFFFAOYSA-N

Formula: C18H22Cl2O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-281.13	kJ/mol	Joback Method
hf	-688.36	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.048		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	890.20	K	Joback Method
tc	1120.39	K	Joback Method
tf	551.38	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.29	J/mol×K	890.20	Joback Method
cpg	824.42	J/mol×K	928.56	Joback Method
cpg	837.02	J/mol×K	966.93	Joback Method
cpg	848.11	J/mol×K	1005.29	Joback Method
cpg	857.71	J/mol×K	1043.66	Joback Method
cpg	865.83	J/mol×K	1082.02	Joback Method
cpg	872.49	J/mol×K	1120.39	Joback Method
dvisc	0.0005472	Pa×s	551.38	Joback Method

dvisc	0.0003362	Pa×s	607.85	Joback Method
dvisc	0.0002243	Pa×s	664.32	Joback Method
dvisc	0.0001595	Pa×s	720.79	Joback Method
dvisc	0.0001192	Pa×s	777.26	Joback Method
dvisc	0.0000926	Pa×s	833.73	Joback Method
dvisc	0.0000743	Pa×s	890.20	Joback Method

Sources

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=U339843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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