1,2-Cyclohexanedicarboxylic acid, butyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C18H21Cl3O4/c1-2-3-8-24-17(22)12-6-4-5-7-13(12)18(23)25-16-14(20)9-11(19

InchiKey: UYPZKMWMOWGLMA-UHFFFAOYSA-N

Formula: C18H21Cl3O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	-302.69	kJ/mol	Joback Method
hf	-715.57	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.702		Crippen Method
mcvol	281.460	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2681.00		NIST Webbook
rinpol	2681.00		NIST Webbook
tb	932.61	K	Joback Method
tc	1166.90	K	Joback Method
tf	593.82	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.53	J/mol×K	932.61	Joback Method
cpg	877.89	J/mol×K	1127.85	Joback Method
cpg	871.69	J/mol×K	1088.80	Joback Method
cpg	863.97	J/mol×K	1049.75	Joback Method
cpg	854.71	J/mol×K	1010.71	Joback Method
cpg	843.90	J/mol×K	971.66	Joback Method
cpg	882.57	J/mol×K	1166.90	Joback Method
dvisc	0.0000652	Pa×s	932.61	Joback Method

dvisc	0.0000803	Pa×s	876.14	Joback Method
dvisc	0.0001018	Pa×s	819.68	Joback Method
dvisc	0.0001336	Pa×s	763.22	Joback Method
dvisc	0.0001831	Pa×s	706.75	Joback Method
dvisc	0.0002651	Pa×s	650.29	Joback Method
dvisc	0.0004118	Pa×s	593.82	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=U339808&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