

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

Inchi:	InChI=1S/C18H23ClO4/c1-12(2)11-22-17(20)15-8-3-4-9-16(15)18(21)23-14-7-5-6-13(19)
InchiKey:	KTECVHABHIPEJX-UHFFFAOYSA-N
Formula:	C18H23ClO4
SMILES:	CC(C)COC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	338.83

Physical Properties

Property code	Value	Unit	Source
gf	-262.01	kJ/mol	Joback Method
hf	-666.43	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	81.03	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.251		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
tb	847.35	K	Joback Method
tc	1076.90	K	Joback Method
tf	493.94	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.06	J/molxK	847.35	Joback Method
cpg	803.15	J/molxK	885.61	Joback Method
cpg	817.66	J/molxK	923.87	Joback Method
cpg	830.63	J/molxK	962.12	Joback Method
cpg	842.09	J/molxK	1000.38	Joback Method
cpg	852.04	J/molxK	1038.64	Joback Method
cpg	860.52	J/molxK	1076.90	Joback Method
dvisc	0.0008267	Paxs	493.94	Joback Method
dvisc	0.0004510	Paxs	552.84	Joback Method
dvisc	0.0002765	Paxs	611.74	Joback Method

dvisc	0.0001847	Paxs	670.64	Joback Method
dvisc	0.0001317	Paxs	729.55	Joback Method
dvisc	0.0000988	Paxs	788.45	Joback Method
dvisc	0.0000771	Paxs	847.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U339692&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

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