

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

Inchi:	InChI=1S/C17H21ClO4/c1-2-10-21-16(19)14-8-3-4-9-15(14)17(20)22-13-7-5-6-12(18)11-
InchiKey:	QSVCXDSXLXGQPS-UHFFFAOYSA-N
Formula:	C17H21ClO4
SMILES:	CCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	324.80

Physical Properties

Property code	Value	Unit	Source
gf	-267.99	kJ/mol	Joback Method
hf	-640.51	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.005		Crippen Method
mvol	242.890	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	824.91	K	Joback Method
tc	1053.94	K	Joback Method
tf	497.67	K	Joback Method
vc	0.908	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.03	J/molxK	824.91	Joback Method
cpg	793.83	J/molxK	1015.77	Joback Method
cpg	783.78	J/molxK	977.60	Joback Method
cpg	772.29	J/molxK	939.42	Joback Method
cpg	759.35	J/molxK	901.25	Joback Method
cpg	744.93	J/molxK	863.08	Joback Method
cpg	802.47	J/molxK	1053.94	Joback Method
dvisc	0.0000961	Paxs	824.91	Joback Method

dvisc	0.0001210	Paxs	770.37	Joback Method
dvisc	0.0001577	Paxs	715.83	Joback Method
dvisc	0.0002147	Paxs	661.29	Joback Method
dvisc	0.0003089	Paxs	606.75	Joback Method
dvisc	0.0004777	Paxs	552.21	Joback Method
dvisc	0.0008127	Paxs	497.67	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=U339691&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

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