

1,2-Cyclohexanedicarboxylic acid, 2-chlorophenyl pentyl ester

Inchi:	InChI=1S/C19H25ClO4/c1-2-3-8-13-23-18(21)14-9-4-5-10-15(14)19(22)24-17-12-7-6-11
InchiKey:	KPLPMJGMUYNOAR-UHFFFAOYSA-N
Formula:	C19H25ClO4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	352.85

Physical Properties

Property code	Value	Unit	Source
gf	-251.15	kJ/mol	Joback Method
hf	-681.79	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.785		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	870.67	K	Joback Method
tc	1094.87	K	Joback Method
tf	520.21	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.76	J/molxK	870.67	Joback Method
cpg	860.57	J/molxK	908.04	Joback Method
cpg	874.86	J/molxK	945.40	Joback Method
cpg	887.64	J/molxK	982.77	Joback Method
cpg	898.94	J/molxK	1020.14	Joback Method
cpg	908.79	J/molxK	1057.50	Joback Method
cpg	917.20	J/molxK	1094.87	Joback Method
dvisc	0.0006746	Paxs	520.21	Joback Method

dvisc	0.0003868	Paxs	578.62	Joback Method
dvisc	0.0002456	Paxs	637.03	Joback Method
dvisc	0.0001683	Paxs	695.44	Joback Method
dvisc	0.0001223	Paxs	753.85	Joback Method
dvisc	0.0000930	Paxs	812.26	Joback Method
dvisc	0.0000734	Paxs	870.67	Joback Method

Sources

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=U339585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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