

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

Inchi:	InChI=1S/C20H27ClO4/c1-2-3-4-9-14-24-19(22)15-10-5-6-11-16(15)20(23)25-18-13-8-7
InchiKey:	WMJNGNFTCBUQKK-UHFFFAOYSA-N
Formula:	C20H27ClO4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	366.88

Physical Properties

Property code	Value	Unit	Source
gf	-242.73	kJ/mol	Joback Method
hf	-702.43	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	85.87	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.175		Crippen Method
mvol	285.160	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2596.00		NIST Webbook
tb	893.55	K	Joback Method
tc	1116.35	K	Joback Method
tf	531.48	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.66	J/molxK	893.55	Joback Method
cpg	919.39	J/molxK	930.68	Joback Method
cpg	933.57	J/molxK	967.82	Joback Method
cpg	946.22	J/molxK	1004.95	Joback Method
cpg	957.38	J/molxK	1042.08	Joback Method
cpg	967.07	J/molxK	1079.22	Joback Method
cpg	975.31	J/molxK	1116.35	Joback Method
dvisc	0.0006106	Paxs	531.48	Joback Method
dvisc	0.0003460	Paxs	591.83	Joback Method

dvisc	0.0002178	Paxs	652.17	Joback Method
dvisc	0.0001483	Paxs	712.51	Joback Method
dvisc	0.0001072	Paxs	772.86	Joback Method
dvisc	0.0000812	Paxs	833.20	Joback Method
dvisc	0.0000639	Paxs	893.55	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=U339587&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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