1,2-Cyclohexanedicarboxylic acid, 2,5-dichlorophenyl propyl ester

Inchi: InChI=1S/C17H20Cl2O4/c1-2-9-22-16(20)12-5-3-4-6-13(12)17(21)23-15-10-11(18)7-8-14

InchiKey: JFGWRJVIDRNNTK-UHFFFAOYSA-N

Formula: C17H20Cl2O4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 359.24

Physical Properties

Property code	Value	Unit	Source
gf	-289.55	kJ/mol	Joback Method
hf	-667.72	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	84.24	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.658		Crippen Method
mcvol	255.130	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	867.32	K	Joback Method
tc	1099.89	K	Joback Method
tf	540.11	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.80	J/mol×K	867.32	Joback Method
cpg	766.97	J/mol×K	906.08	Joback Method
cpg	779.63	J/mol×K	944.84	Joback Method
cpg	790.80	J/mol×K	983.61	Joback Method
cpg	800.50	J/mol×K	1022.37	Joback Method
cpg	808.73	J/mol×K	1061.13	Joback Method
cpg	815.51	J/mol×K	1099.89	Joback Method
dvisc	0.0006022	Pa×s	540.11	Joback Method

dvisc	0.0003745	Pa×s	594.64	Joback Method
dvisc	0.0002522	Pa×s	649.18	Joback Method
dvisc	0.0001806	Pa×s	703.71	Joback Method
dvisc	0.0001357	Pa×s	758.25	Joback Method
dvisc	0.0001059	Pa×s	812.78	Joback Method
dvisc	0.0000853	Pa×s	867.32	Joback Method

Sources

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=U339796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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