1,2-Cyclohexanedicarboxylic acid, 2,3-dichlorophenyl pentyl ester

Inchi: InChI=1S/C19H24Cl2O4/c1-2-3-6-12-24-18(22)13-8-4-5-9-14(13)19(23)25-16-11-7-10-15

InchiKey: ZPDABEFERPPTQQ-UHFFFAOYSA-N

Formula: C19H24Cl2O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 387.30

Physical Properties

Property code	Value	Unit	Source
gf	-272.71	kJ/mol	Joback Method
hf	-709.00	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	88.69	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.439		Crippen Method
mcvol	283.310	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2688.00		NIST Webbook
rinpol	2688.00		NIST Webbook
tb	913.08	K	Joback Method
tc	1141.60	K	Joback Method
tf	562.65	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.44	J/mol×K	913.08	Joback Method
cpg	923.41	J/mol×K	1103.51	Joback Method
cpg	915.45	J/mol×K	1065.42	Joback Method
cpg	905.99	J/mol×K	1027.34	Joback Method
cpg	895.01	J/mol×K	989.25	Joback Method
cpg	882.50	J/mol×K	951.17	Joback Method
cpg	929.91	J/mol×K	1141.60	Joback Method
dvisc	0.0000646	Pa×s	913.08	Joback Method

dvisc	0.0000808	Pa×s	854.67	Joback Method
dvisc	0.0001044	Pa×s	796.27	Joback Method
dvisc	0.0001404	Pa×s	737.87	Joback Method
dvisc	0.0001989	Pa×s	679.46	Joback Method
dvisc	0.0003006	Pa×s	621.05	Joback Method
dvisc	0.0004952	Pa×s	562.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U339844&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