1,2-Cyclohexanedicarboxylic acid, octyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C22H29Cl3O4/c1-2-3-4-5-6-9-12-28-21(26)16-10-7-8-11-17(16)22(27)29-20-18

InchiKey: ODBKFGMQBCKILK-UHFFFAOYSA-N

Formula: C22H29Cl3O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 463.82

Physical Properties

Property code	Value	Unit	Source
gf	-269.01	kJ/mol	Joback Method
hf	-798.13	kJ/mol	Joback Method
hfus	56.68	kJ/mol	Joback Method
hvap	100.41	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.262		Crippen Method
mcvol	337.820	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	3087.00		NIST Webbook
rinpol	3087.00		NIST Webbook
tb	1024.13	K	Joback Method
tc	1258.83	K	Joback Method
tf	638.90	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.50	J/mol×K	1024.13	Joback Method
cpg	1078.43	J/mol×K	1063.25	Joback Method
cpg	1088.62	J/mol×K	1102.36	Joback Method
cpg	1097.09	J/mol×K	1141.48	Joback Method
cpg	1103.89	J/mol×K	1180.60	Joback Method
cpg	1109.03	J/mol×K	1219.71	Joback Method
cpg	1112.55	J/mol×K	1258.83	Joback Method
dvisc	0.0002664	Pa×s	638.90	Joback Method

dvisc	0.0001641	Pa×s	703.11	Joback Method
dvisc	0.0001097	Pa×s	767.31	Joback Method
dvisc	0.0000780	Pa×s	831.52	Joback Method
dvisc	0.0000582	Pa×s	895.72	Joback Method
dvisc	0.0000452	Pa×s	959.93	Joback Method
dvisc	0.0000362	Pa×s	1024.13	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=U339813&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