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

Inchi: InChI=1S/C20H25Cl3O4/c1-12(2)6-5-9-26-19(24)14-7-3-4-8-15(14)20(25)27-18-16(22)10

InchiKey: JODHDCLIOXBAQB-UHFFFAOYSA-N

Formula: C20H25Cl3O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 435.77

Physical Properties

Property code	Value	Unit	Source
gf	-288.29	kJ/mol	Joback Method
hf	-762.13	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	95.58	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.338		Crippen Method
mcvol	309.640	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
tb	977.93	K	Joback Method
tc	1212.74	K	Joback Method
tf	601.36	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.52	J/mol×K	977.93	Joback Method
cpg	960.75	J/mol×K	1017.06	Joback Method
cpg	971.29	J/mol×K	1056.20	Joback Method
cpg	980.18	J/mol×K	1095.33	Joback Method
cpg	987.43	J/mol×K	1134.47	Joback Method
cpg	993.06	J/mol×K	1173.60	Joback Method
cpg	997.10	J/mol×K	1212.74	Joback Method
dvisc	0.0003533	Pa×s	601.36	Joback Method

dvisc	0.0002124	Pa×s	664.12	Joback Method
dvisc	0.0001394	Pa×s	726.88	Joback Method
dvisc	0.0000979	Pa×s	789.64	Joback Method
dvisc	0.0000724	Pa×s	852.41	Joback Method
dvisc	0.0000558	Pa×s	915.17	Joback Method
dvisc	0.0000444	Pa×s	977.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339810&Units=SI
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

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