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

Inchi: InChI=1S/C19H23Cl3O4/c1-2-3-6-9-25-18(23)13-7-4-5-8-14(13)19(24)26-17-15(21)10-12

InchiKey: PCSYOVGAUYFPPK-UHFFFAOYSA-N

Formula: C19H23Cl3O4

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

Mol. weight [g/mol]: 421.74

Physical Properties

Property code	Value	Unit	Source
gf	-294.27	kJ/mol	Joback Method
hf	-736.21	kJ/mol	Joback Method
hfus	48.91	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.092		Crippen Method
mcvol	295.550	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2774.00		NIST Webbook
rinpol	2774.00		NIST Webbook
tb	955.49	K	Joback Method
tc	1188.60	K	Joback Method
tf	605.09	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.55	J/mol×K	955.49	Joback Method
cpg	935.19	J/mol×K	1149.75	Joback Method
cpg	929.19	J/mol×K	1110.90	Joback Method
cpg	921.64	J/mol×K	1072.04	Joback Method
cpg	912.53	J/mol×K	1033.19	Joback Method
cpg	901.84	J/mol×K	994.34	Joback Method
cpg	939.66	J/mol×K	1188.60	Joback Method
dvisc	0.0000565	Pa×s	955.49	Joback Method

dvisc	0.0000698	Pa×s	897.09	Joback Method
dvisc	0.0000888	Pa×s	838.69	Joback Method
dvisc	0.0001172	Pa×s	780.29	Joback Method
dvisc	0.0001617	Pa×s	721.89	Joback Method
dvisc	0.0002362	Pa×s	663.49	Joback Method
dvisc	0.0003711	Pa×s	605.09	Joback Method

Sources

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=U339809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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