Cyclohexanecarboxylic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C13H12Cl4O2/c14-8-6-9(15)12(11(17)10(8)16)19-13(18)7-4-2-1-3-5-7/h6-7H,1

InchiKey: RXIUUOITUXXFKV-UHFFFAOYSA-N

Formula: C13H12Cl4O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)C1CCCCC1

Mol. weight [g/mol]: 342.05

Physical Properties

Property code	Value	Unit	Source
gf	-124.72	kJ/mol	Joback Method
hf	-374.44	kJ/mol	Joback Method
hfus	33.32	kJ/mol	Joback Method
hvap	76.58	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.786		Crippen Method
mcvol	215.810	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2323.00		NIST Webbook
tb	789.00	K	Joback Method
tc	1041.77	K	Joback Method
tf	511.99	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.13	J/mol×K	789.00	Joback Method
cpg	584.94	J/mol×K	999.64	Joback Method
cpg	576.98	J/mol×K	957.51	Joback Method
cpg	567.84	J/mol×K	915.38	Joback Method
cpg	557.51	J/mol×K	873.26	Joback Method
cpg	545.94	J/mol×K	831.13	Joback Method
cpg	591.74	J/mol×K	1041.77	Joback Method
dvisc	0.0001210	Pa×s	789.00	Joback Method
dvisc	0.0001478	Pa×s	742.83	Joback Method

dvisc	0.0001854	Pa×s	696.66	Joback Method
dvisc	0.0002402	Pa×s	650.50	Joback Method
dvisc	0.0003237	Pa×s	604.33	Joback Method
dvisc	0.0004583	Pa×s	558.16	Joback Method
dvisc	0.0006909	Pa×s	511.99	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=U354654&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