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

Inchi: InChI=1S/C12H11Cl5O2/c13-5-3-1-2-4-9(18)19-12-8(15)6-7(14)10(16)11(12)17/h6H,1-5

InchiKey: UAAXZIFBHCXCQB-UHFFFAOYSA-N

Formula: C12H11Cl5O2

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

Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-169.52	kJ/mol	Joback Method
hf	-423.86	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	78.31	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	6.005		Crippen Method
mcvol	224.820	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2446.00		NIST Webbook
tb	784.00	K	Joback Method
tc	1009.78	K	Joback Method
tf	523.26	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.72	J/mol×K	784.00	Joback Method
cpg	520.48	J/mol×K	821.63	Joback Method
cpg	529.48	J/mol×K	859.26	Joback Method
cpg	537.73	J/mol×K	896.89	Joback Method
cpg	545.25	J/mol×K	934.52	Joback Method
cpg	552.04	J/mol×K	972.15	Joback Method
cpg	558.12	J/mol×K	1009.78	Joback Method
dvisc	0.0005637	Pa×s	523.26	Joback Method
dvisc	0.0003912	Pa×s	566.72	Joback Method

dvisc	0.0002859	Pa×s	610.17	Joback Method
dvisc	0.0002179	Pa×s	653.63	Joback Method
dvisc	0.0001718	Pa×s	697.09	Joback Method
dvisc	0.0001393	Pa×s	740.54	Joback Method
dvisc	0.0001155	Pa×s	784.00	Joback Method

Sources

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=U354732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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