

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

Inchi:	InChI=1S/C14H14Cl4O2/c15-9-7-10(16)14(13(18)12(9)17)20-11(19)6-5-8-3-1-2-4-8/h7-8
InchiKey:	UJTJVNOPSZRYPT-UHFFFAOYSA-N
Formula:	C14H14Cl4O2
SMILES:	O=C(CCC1CCCC1)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	356.07

Physical Properties

Property code	Value	Unit	Source
gf	-104.20	kJ/mol	Joback Method
hf	-388.92	kJ/mol	Joback Method
hfus	38.01	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.176		Crippen Method
mcvol	229.900	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinsol	2422.00		NIST Webbook
tb	807.61	K	Joback Method
tc	1048.64	K	Joback Method
tf	526.78	K	Joback Method
vc	0.873	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.91	J/molxK	807.61	Joback Method
cpg	596.57	J/molxK	847.78	Joback Method
cpg	608.13	J/molxK	887.95	Joback Method
cpg	618.62	J/molxK	928.12	Joback Method
cpg	628.06	J/molxK	968.30	Joback Method
cpg	636.51	J/molxK	1008.47	Joback Method
cpg	643.99	J/molxK	1048.64	Joback Method
dvisc	0.0007443	Paxs	526.78	Joback Method
dvisc	0.0005115	Paxs	573.59	Joback Method

dvisc	0.0003720	Paxs	620.39	Joback Method
dvisc	0.0002829	Paxs	667.20	Joback Method
dvisc	0.0002230	Paxs	714.00	Joback Method
dvisc	0.0001810	Paxs	760.81	Joback Method
dvisc	0.0001505	Paxs	807.61	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=U354060&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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