

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

Inchi:	InChI=1S/C10H7Cl5O2/c11-3-1-2-7(16)17-10-6(13)4-5(12)8(14)9(10)15/h4H,1-3H2
InchiKey:	WFRIAUUGCHUAOK-UHFFFAOYSA-N
Formula:	C10H7Cl5O2
SMILES:	O=C(CCCCl)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	336.43

Physical Properties

Property code	Value	Unit	Source
gf	-186.36	kJ/mol	Joback Method
hf	-382.58	kJ/mol	Joback Method
hfus	37.91	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.225		Crippen Method
mcvol	196.640	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinsol	2151.00		NIST Webbook
tb	738.24	K	Joback Method
tc	971.65	K	Joback Method
tf	500.72	K	Joback Method
vc	0.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.07	J/molxK	738.24	Joback Method
cpg	444.85	J/molxK	932.75	Joback Method
cpg	439.01	J/molxK	893.85	Joback Method
cpg	432.52	J/molxK	854.94	Joback Method
cpg	425.37	J/molxK	816.04	Joback Method
cpg	417.55	J/molxK	777.14	Joback Method
cpg	450.04	J/molxK	971.65	Joback Method
dvisc	0.0001498	Paxs	738.24	Joback Method
dvisc	0.0001788	Paxs	698.65	Joback Method

dvisc	0.0002180	Paxs	659.07	Joback Method
dvisc	0.0002727	Paxs	619.48	Joback Method
dvisc	0.0003515	Paxs	579.89	Joback Method
dvisc	0.0004704	Paxs	540.31	Joback Method
dvisc	0.0006591	Paxs	500.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U360646&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

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