

1-(2-Chloroethoxy)-2-(2,2,4,6-tetrachlorophenoxy)ethane

Inchi:	InChI=1S/C10H9Cl5O2/c11-1-2-16-3-4-17-10-7(13)5-6(12)8(14)9(10)15/h5H,1-4H2
InchiKey:	MUFFSGFNYHDFMP-UHFFFAOYSA-N
Formula:	C10H9Cl5O2
SMILES:	CICCOCCOc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	338.44
CAS:	5335-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-162.44	kJ/mol	Joback Method
hf	-402.22	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.934		Crippen Method
mcvol	200.940	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
tb	706.79	K	Joback Method
tc	931.61	K	Joback Method
tf	473.02	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.93	J/molxK	706.79	Joback Method
cpg	466.81	J/molxK	894.14	Joback Method
cpg	459.77	J/molxK	856.67	Joback Method
cpg	452.06	J/molxK	819.20	Joback Method
cpg	443.68	J/molxK	781.73	Joback Method
cpg	434.63	J/molxK	744.26	Joback Method
cpg	473.15	J/molxK	931.61	Joback Method
dvisc	0.0001149	Paxs	706.79	Joback Method
dvisc	0.0001375	Paxs	667.83	Joback Method

dvisc	0.0001684	Paxs	628.87	Joback Method
dvisc	0.0002118	Paxs	589.90	Joback Method
dvisc	0.0002750	Paxs	550.94	Joback Method
dvisc	0.0003717	Paxs	511.98	Joback Method
dvisc	0.0005280	Paxs	473.02	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=C5335262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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