Chloroacetic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C7H5ClF8O2/c8-1-3(17)18-2-5(11,12)7(15,16)6(13,14)4(9)10/h4H,1-2H2

InchiKey: SPDQTHCMRQYIIW-UHFFFAOYSA-N

Formula: C7H5ClF8O2

SMILES: O=C(CCl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 308.55

Physical Properties

Property code	Value	Unit	Source
gf	-1790.19	kJ/mol	Joback Method
hf	-2048.76	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	33.91	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.939		Crippen Method
mcvol	143.330	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1018.00		NIST Webbook
tb	457.31	K	Joback Method
tc	607.93	K	Joback Method
tf	267.71	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.43	J/mol×K	457.31	Joback Method
cpg	350.53	J/mol×K	482.41	Joback Method
cpg	360.01	J/mol×K	507.52	Joback Method
cpg	368.88	J/mol×K	532.62	Joback Method
cpg	377.19	J/mol×K	557.72	Joback Method
cpg	384.95	J/mol×K	582.83	Joback Method
cpg	392.18	J/mol×K	607.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354602&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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