3,5,7,8-Tetrachloro-2,2,3,4,4,5,6,6,7,8,8-undecafluo octanoic acid

Inchi: InChI=1S/C8HCl4F11O2/c9-3(15,2(13,14)1(24)25)6(18,19)4(10,16)7(20,21)5(11,17)8(12
InchiKey: YSPJDMQUTGFRFK-UHFFFAOYSA-N
Formula: C8HCl4F11O2
SMILES: O=C(O)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)Cl
Mol. weight [g/mol]: 479.89
CAS: 2923-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-2420.01	kJ/mol	Joback Method
hf	-2754.68	kJ/mol	Joback Method
hfus	20.93	kJ/mol	Joback Method
hvap	56.31	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.522		Crippen Method
mcvol	199.450	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
tb	647.57	K	Joback Method
tc	818.26	K	Joback Method
tf	433.78	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.53	J/mol×K	647.57	Joback Method
cpg	526.50	J/mol×K	676.02	Joback Method
cpg	531.67	J/mol×K	704.47	Joback Method
cpg	536.13	J/mol×K	732.92	Joback Method
cpg	539.97	J/mol×K	761.36	Joback Method
cpg	543.29	J/mol×K	789.81	Joback Method
cpg	546.18	J/mol×K	818.26	Joback Method
hvapt	70.60	kJ/mol	463.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2923684&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume