3,5,6-Trichloro-2,2,3,4,4,5,6,6-octafluorohexanoic acid

Inchi: InChI=1S/C6HCl3F8O2/c7-3(12,2(10,11)1(18)19)5(14,15)4(8,13)6(9,16)17/h(H,18,19)
InchiKey: ANRGSWRBGXZQLY-UHFFFAOYSA-N
Formula: C6HCl3F8O2
SMILES: O=C(O)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)Cl
Mol. weight [g/mol]: 363.42
CAS: 2106-54-9

Physical Properties

Property code	Value	Unit	Source
gf	-1846.17	kJ/mol	Joback Method
hf	-2091.83	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.982		Crippen Method
mcvol	153.720	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	573.03	K	Joback Method
tc	744.30	K	Joback Method
tf	374.71	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.76	J/mol×K	573.03	Joback Method
cpg	384.30	J/mol×K	601.58	Joback Method
cpg	390.05	J/mol×K	630.12	Joback Method
cpg	395.10	J/mol×K	658.67	Joback Method
cpg	399.51	J/mol×K	687.21	Joback Method
cpg	403.34	J/mol×K	715.76	Joback Method
cpg	406.67	J/mol×K	744.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.99042e+01
Coeff. B	-7.72168e+03
Temperature range (K), min.	373.00
Temperature range (K), max.	529.14

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003897&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume