3,5,7,9,10-Pentachloro-2,2,3,4,4,5,6,6,7,8,8,9,10,10 acid

Other names: 2,2,3,4,4,5,6,6,7,8,8,9,10,10-Tetradecafluoro-3,5,7,9,10-pentachlorodecanoic acid

Inchi: InChI=1S/C10HCl5F14O2/c11-3(18,2(16,17)1(30)31)7(22,23)4(12,19)8(24,25)5(13,20)9(

InchiKey: ADMOCDJEQJUWJY-UHFFFAOYSA-N

Formula: C10HCl5F14O2

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)C(F)(Cl)C(F)(F)Cl

Mol. weight [g/mol]: 596.36

CAS: 335-74-0

Physical Properties

Property code	Value	Unit	Source
gf	-2993.85	kJ/mol	Joback Method
hf	-3417.53	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	60.10	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	7.062		Crippen Method
mcvol	245.180	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
tb	722.11	K	Joback Method
tc	895.52	K	Joback Method
tf	492.85	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.90	J/mol×K	722.11	Joback Method
cpg	669.88	J/mol×K	751.01	Joback Method
cpg	674.14	J/mol×K	779.91	Joback Method
cpg	677.82	J/mol×K	808.81	Joback Method
cpg	681.03	J/mol×K	837.71	Joback Method
cpg	683.90	J/mol×K	866.62	Joback Method
cpg	686.57	J/mol×K	895.52	Joback Method
hvapt	80.60	kJ/mol	475.50	NIST Webbook

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=C335740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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