3,4-Dichloro-2,2,3,4,4-pentaflurobutyric acid

Other names: 3,4-Dichloro-2,2,3,4,4-pentafluorobutyric acid
Inchi: InChI=1S/C4HCl2F5O2/c5-3(9,4(6,10)11)2(7,8)1(12)13/h(H,12,13)
InchiKey: WVWCLNDERHVFSB-UHFFFAOYSA-N
Formula: C4HCl2F5O2
SMILES: O=C(O)C(F)(F)C(F)(Cl)C(F)(F)Cl
Mol. weight [g/mol]: 246.95
CAS: 375-07-5

Physical Properties

Property code	Value	Unit	Source
gf	-1272.33	kJ/mol	Joback Method
hf	-1428.98	kJ/mol	Joback Method
hfus	13.35	kJ/mol	Joback Method
hvap	48.72	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.443		Crippen Method
mcvol	107.990	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	498.49	K	Joback Method
tc	671.96	K	Joback Method
tf	315.64	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.72	J/mol×K	498.49	Joback Method
cpg	246.80	J/mol×K	527.40	Joback Method
cpg	252.25	J/mol×K	556.31	Joback Method
cpg	257.14	J/mol×K	585.23	Joback Method
cpg	261.48	J/mol×K	614.14	Joback Method
cpg	265.34	J/mol×K	643.05	Joback Method
cpg	268.75	J/mol×K	671.96	Joback Method
hvapt	54.80	kJ/mol	414.50	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=C375075&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