1,1,1,3-tetrachlorotetrafluoropropane

Inchi: InChI=1S/C3Cl4F4/c4-2(5,6)1(8,9)3(7,10)11
InchiKey: IQJADVFBZGJGSI-UHFFFAOYSA-N
Formula: C3Cl4F4
SMILES: FC(F)(Cl)C(F)(F)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 253.84
CAS: 2268-46-4

Physical Properties

Property code	Value	Unit	Source
gf	-844.06	kJ/mol	Joback Method
hf	-978.90	kJ/mol	Joback Method
hfus	10.39	kJ/mol	Joback Method
hvap	32.66	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.824		Crippen Method
mcvol	109.170	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	387.00	K	NIST Webbook
tb	387.70 ± 0.60	K	NIST Webbook
tc	599.84	K	Joback Method
tf	252.87	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.94	J/mol×K	405.15	Joback Method
cpg	198.20	J/mol×K	437.60	Joback Method
cpg	204.60	J/mol×K	470.05	Joback Method
cpg	210.20	J/mol×K	502.49	Joback Method
cpg	215.06	J/mol×K	534.94	Joback Method
cpg	219.23	J/mol×K	567.39	Joback Method
cpg	222.79	J/mol×K	599.84	Joback Method

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=C2268464&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
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