Heptafluorobutyryl chloride

Other names:	Perfluorobutyryl chloride
	Butanoyl chloride, heptafluoro-
Inchi:	InChI=1S/C4ClF7O/c5-1(13)2(6,7)3(8,9)4(10,11)12
InchiKey:	WFELVFKXQJYPSL-UHFFFAOYSA-N
Formula:	C4ClF7O
SMILES:	O=C(Cl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	232.48
CAS:	375-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-1513.20	kJ/mol	Joback Method
hf	-1653.23	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	26.02	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.585		Crippen Method
mcvol	93.420	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	311.50 ± 0.50	K	NIST Webbook
tb	311.70	K	NIST Webbook
tc	522.07	K	Joback Method
tf	226.08	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.94	J/mol×K	367.42	Joback Method
cpg	202.21	J/mol×K	393.19	Joback Method
cpg	209.85	J/mol×K	418.97	Joback Method
cpg	216.87	J/mol×K	444.74	Joback Method
cpg	223.31	J/mol×K	470.52	Joback Method
cpg	229.20	J/mol×K	496.29	Joback Method

cpg	234.57	J/mol×K	522.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375166&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
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