Perfluorooctanoyl chloride

Other names:	Octanoyl chloride, pentadecafluoro-
	Perfluorooctanoic acid chloride
	Perfluorocaprylic chloride
	n-Perfluorooctanoyl chloride
	Pentadecafluorooctanoyl chloride
	pentadecafluorooctyl chloride
Inchi:	InChI=1S/C8ClF15O/c9-1(25)2(10,11)3(12,13)4(14,15)5(16,17)6(18,19)7(20,21)8(22,23)
InchiKey:	AQQBRCXWZZAFOK-UHFFFAOYSA-N
Formula:	C8ClF15O
SMILES:	O=C(Cl)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	432.51
CAS:	335-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-3026.64	kJ/mol	Joback Method
hf	-3339.67	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	23.21	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.126		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
tb	404.00 ± 1.00	K	NIST Webbook
tc	573.05	K	Joback Method
tf	285.56	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.86	J/mol×K	440.18	Joback Method
cpg	436.60	J/mol×K	462.32	Joback Method
cpg	447.43	J/mol×K	484.47	Joback Method

cpg	457.39	J/mol×K	506.61	Joback Method
cpg	466.52	J/mol×K	528.76	Joback Method
cpg	474.87	J/mol×K	550.90	Joback Method
cpg	482.49	J/mol×K	573.05	Joback Method

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=C335648&Units=SI

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