PERFLUOROOCTANOYL CHLORIDE

Other names:	Octanoyl chloride, pentadecafluoro-
	Pentadecafluorooctanoyl chloride
	Perfluorocaprylic chloride
	Perfluorooctanoic acid chloride
	n-Perfluorooctanoyl 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)C(F)(F)F
Mol. weight [g/mol]:	432.51

Physical Properties

Property code	Value	Unit	Source
af	0.5427		Cheméo Relay (1.0)
gf	-3026.64	kJ/mol	Joback Method
hf	-3364.47	kJ/mol	Cheméo Relay (1.0)
hfus	16.57	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Cheméo Relay (1.0)
ie	11.20	eV	Cheméo Relay (1.0)
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	548.84	K	Cheméo Relay (1.0)
tf	284.51	K	Cheméo Relay (1.0)
vc	0.693	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C335648&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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

ie: Ionization energy

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