Dodecafluoro-(2-methyl-3-oxahexanoyl) fluoride

Inchi: InChI=1S/C6F12O2/c7-1(19)2(8,4(11,12)13)20-6(17,18)3(9,10)5(14,15)16
InchiKey: BCLQALQSEBVVAD-UHFFFAOYSA-N
Formula: C6F12O2
SMILES: O=C(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 332.04
CAS: 75566-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-2557.80	kJ/mol	Joback Method
hf	-2809.04	kJ/mol	Joback Method
hfus	13.97	kJ/mol	Joback Method
hvap	21.82	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.518		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	328.00 ± 1.00	K	NIST Webbook
tc	518.32	K	Joback Method
tf	248.72	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.03	J/mol×K	388.06	Joback Method
cpg	317.34	J/mol×K	409.77	Joback Method
cpg	326.98	J/mol×K	431.48	Joback Method
cpg	335.98	J/mol×K	453.19	Joback Method
cpg	344.37	J/mol×K	474.90	Joback Method
cpg	352.16	J/mol×K	496.61	Joback Method
cpg	359.39	J/mol×K	518.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75566608&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