8-Chloro-1-octanol, chlorodifluoroacetate

Inchi: InChI=1S/C10H16Cl2F2O2/c11-7-5-3-1-2-4-6-8-16-9(15)10(12,13)14/h1-8H2
InchiKey: PIBBNTFUMNNFPP-UHFFFAOYSA-N
Formula: C10H16Cl2F2O2
SMILES: O=C(OCCCCCCCCCCl)C(F)(F)Cl
Mol. weight [g/mol]: 277.14

Physical Properties

Property code	Value	Unit	Source
gf	-611.24	kJ/mol	Joback Method
hf	-926.98	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.941		Crippen Method
mcvol	187.220	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1504.00		NIST Webbook
tb	574.66	K	Joback Method
tc	750.74	K	Joback Method
tf	338.06	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.05	J/mol×K	574.66	Joback Method
cpg	459.59	J/mol×K	604.01	Joback Method
cpg	471.49	J/mol×K	633.35	Joback Method
cpg	482.76	J/mol×K	662.70	Joback Method
cpg	493.44	J/mol×K	692.05	Joback Method
cpg	503.54	J/mol×K	721.39	Joback Method
cpg	513.09	J/mol×K	750.74	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=U376213&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume