3-Oxypentanol, 5-chloro, heptafluorobutyrate

Inchi: InChI=1S/C8H8ClF7O3/c9-1-2-18-3-4-19-5(17)6(10,11)7(12,13)8(14,15)16/h1-4H2
InchiKey: VFWWIOIQKUUHFJ-UHFFFAOYSA-N
Formula: C8H8ClF7O3
SMILES: O=C(OCCOCCCl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 320.59

Physical Properties

Property code	Value	Unit	Source
gf	-1689.52	kJ/mol	Joback Method
hf	-2000.23	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.618		Crippen Method
mcvol	161.520	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	929.00		NIST Webbook
tb	503.78	K	Joback Method
tc	658.30	K	Joback Method
tf	315.62	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.12	J/mol×K	503.78	Joback Method
cpg	409.71	J/mol×K	529.53	Joback Method
cpg	419.69	J/mol×K	555.29	Joback Method
cpg	429.09	J/mol×K	581.04	Joback Method
cpg	437.93	J/mol×K	606.79	Joback Method
cpg	446.24	J/mol×K	632.54	Joback Method
cpg	454.03	J/mol×K	658.30	Joback Method

Sources

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=U374839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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