3-Oxypentanol, 5-chloro, trifluoroacetate

Inchi: InChI=1S/C6H8ClF3O3/c7-1-2-12-3-4-13-5(11)6(8,9)10/h1-4H2
InchiKey: GMCNAIXEBHZCAY-UHFFFAOYSA-N
Formula: C6H8ClF3O3
SMILES: O=C(OCCOCCCl)C(F)(F)F
Mol. weight [g/mol]: 220.57

Physical Properties

Property code	Value	Unit	Source
gf	-932.80	kJ/mol	Joback Method
hf	-1157.01	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.347		Crippen Method
mcvol	126.260	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	898.00		NIST Webbook
tb	467.40	K	Joback Method
tc	635.32	K	Joback Method
tf	285.88	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.78	J/mol×K	467.40	Joback Method
cpg	283.81	J/mol×K	495.39	Joback Method
cpg	292.46	J/mol×K	523.37	Joback Method
cpg	300.73	J/mol×K	551.36	Joback Method
cpg	308.63	J/mol×K	579.34	Joback Method
cpg	316.15	J/mol×K	607.33	Joback Method
cpg	323.32	J/mol×K	635.32	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=U374838&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