1,4-Dioxane-2,3-diol, chlorodifluoroacetate, trifluoroacetate

Inchi: InChI=1S/C8H6ClF5O6/c9-7(10,11)5(15)19-3-4(18-2-1-17-3)20-6(16)8(12,13)14/h3-4H,1

InchiKey: LFDUQHBYCNNQOV-UHFFFAOYSA-N

Formula: C8H6ClF5O6

SMILES: O=C(OC1OCCOC1OC(=O)C(F)(F)Cl)C(F)(F)F

Mol. weight [g/mol]: 328.57

Physical Properties

Property code	Value	Unit	Source
gf	-1587.16	kJ/mol	Joback Method
hf	-1941.86	kJ/mol	Joback Method
hfus	35.68	kJ/mol	Joback Method
hvap	58.56	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.166		Crippen Method
mcvol	160.430	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1134.00		NIST Webbook
tb	631.12	K	Joback Method
tc	825.93	K	Joback Method
tf	418.23	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.61	J/mol×K	631.12	Joback Method
cpg	453.79	J/mol×K	663.59	Joback Method
cpg	464.13	J/mol×K	696.06	Joback Method
cpg	473.66	J/mol×K	728.52	Joback Method
cpg	482.40	J/mol×K	760.99	Joback Method
cpg	490.38	J/mol×K	793.46	Joback Method
cpg	497.60	J/mol×K	825.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375758&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume