1,4-Dioxane-2,3-diol, bis(chlorodifluoroacetate)

Inchi: InChI=1S/C8H6Cl2F4O6/c9-7(11,12)5(15)19-3-4(18-2-1-17-3)20-6(16)8(10,13)14/h3-4H,
InchiKey: OTKVBLJKNZUMKM-UHFFFAOYSA-N
Formula: C8H6Cl2F4O6
SMILES: O=C(OC1OCCOC1OC(=O)C(F)(F)Cl)C(F)(F)Cl
Mol. weight [g/mol]: 345.03

Physical Properties

Property code	Value	Unit	Source
gf	-1404.28	kJ/mol	Joback Method
hf	-1761.49	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.435		Crippen Method
mcvol	170.900	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
tb	669.28	K	Joback Method
tc	876.18	K	Joback Method
tf	447.56	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.34	J/mol×K	669.28	Joback Method
cpg	468.95	J/mol×K	703.76	Joback Method
cpg	478.66	J/mol×K	738.25	Joback Method
cpg	487.49	J/mol×K	772.73	Joback Method
cpg	495.47	J/mol×K	807.21	Joback Method
cpg	502.63	J/mol×K	841.70	Joback Method
cpg	508.99	J/mol×K	876.18	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=U375753&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

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